

101201

Access DB#

SEARCH REQUEST FORM

Scientific and Technical Information Center

Requester's Full Name: SABHA QAZI Examiner #: 74141 Date: 3/3/06
 Alt Unit: 1616 Phone Number: 30622 Serial Number: 07497, 891
 Mail Box and Bldg Room Location: 4470 Results Format Preferred (circle): PAPER DISK E-MAIL

If more than one search is submitted, please prioritize searches in order of need.

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc. known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

Title of Invention: 16 Hydroxysteroids as selectively active
 Inventors (please provide full names): Keunzer, Hermann, Estrogens
et al.

Earliest Priority Filing Date: 4/27/1995

For Sequence Searches Only Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.

Cl 53 - 65

Please search for the
 Comps 3,16-dihydroxyestra-1,3,5
 (10)-trienes of formula 1 in Cl 1

Please note the substituents $R^{16} + R^{15}$

Specific comps are in Cls 63 + 64

Please see attached sheet

Thank you

STAFF USE ONLY

	Type of Search	Vendors and cost where applicable
Searcher: <u>84</u>	NA Sequence (#)	STN <u>\$1244,50</u>
Searcher Phone #:	AA Sequence (#)	Dialog
Searcher Location:	Structure (#) <u>3</u>	Questel/Orbit
Date Searcher Picked Up: <u>3/16/06</u>	Bibliographic	Dr. Link
Date Completed: <u>3/17/06</u>	Litigation	Lexis/Nexis
Searcher Prep & Review Time: <u>30</u>	Fulltext	Sequence Systems
Clerical Prep Time: <u>30</u>	Patent Family	WWW/Internet
Online Fee: <u>290</u>	Other	Other (specify)

=> d his

(FILE 'HOME' ENTERED AT 08:41:39 ON 17 MAR 2006)

FILE 'HCAPLUS' ENTERED AT 08:41:52 ON 17 MAR 2006

L1 56 S KUENZER H?/AU
L2 14 S KNAUTHE R?/AU
L3 29 S LESSL M?/AU
L4 2 S L1 AND L2 AND L3
L5 79 S FRITZEMEIER K?/AU
L6 10 S BOEMER U?/AU
L7 3628 S MUELLER G?/AU
L8 21 S KOSEMUND D?/AU
L9 1 S L4 AND L5 AND L6 AND L7 AND L8
L10 70 S HEGELE-HARTUNG C?/AU
L11 1 S L10 AND L9
SEL RN

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ACT QAZ891/A

L13 SCR 1844
L14 STR
L15 899 SEA FILE=REGISTRY SSS FUL L14 NOT L13

L16 266 S L12 AND L15
L17 23 S L12 NOT L16

FILE 'LREGISTRY' ENTERED AT 08:59:28 ON 17 MAR 2006

ACT QAZ891A/Q

L18 STR

L19 STR L18

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L21 1 S L20 AND L12

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L23 STR L22

FILE 'REGISTRY' ENTERED AT 10:10:11 ON 17 MAR 2006

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L26 STR L23

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SAV L28 QAZ891A/A
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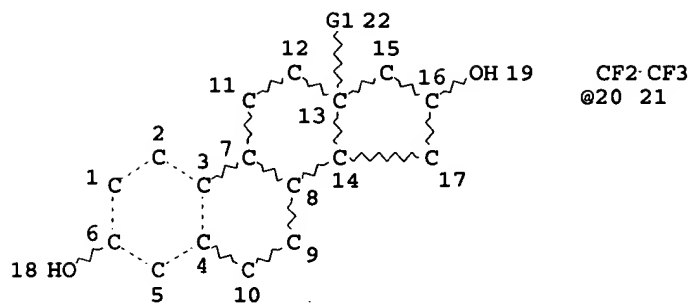
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L36 316 S L32 AND L34

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 L40 410 S L39 AND L31
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 L13 SCR 1844
 L14 STR



VAR G1=ME/ET/CF3/20

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 22

STEREO ATTRIBUTES: NONE

L15 899 SEA FILE=REGISTRY SSS FUL L14 NOT L13

L16 266 SEA FILE=REGISTRY ABB=ON PLU=ON L12 AND L15

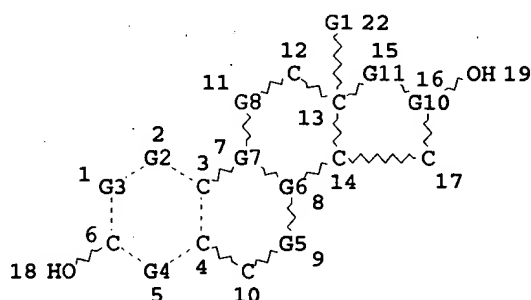
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C~OEt C~Ak C~O~Ak C~CF2-CF3 C~Ak~F
@33 34 @35 36 @37 38 39 @42 41 40 @43 44 45

C~Cy C~CN C~Et C~O~NO2 C~CH2Cl
@46 47 @48 49 @50 51 @52 53 54 @55 56 57

C~G9 C~S~Ak S @62
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C~CH2-CN C~F
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VAR G1=ME/ET/CF3/20

VAR G2=CH/23/27/25/29/31/33

VAR G3=CH/23/27/35/37

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VAR G5=CH/23/35/43/37/46

VAR G6=CH/35/43/48

VAR G7=CH/29/50/25/42

VAR G8=CH2/CH/52/27/58/23/55/35/43/37/46

VAR G9=62/60

VAR G10=CH/35/43/25/42/64

VAR G11=CH2/CH/67/35/43

NODE ATTRIBUTES:

CONNECT IS E2 RC AT 61

CONNECT IS E1 RC AT 62

DEFAULT MLEVEL IS ATOM

GGCAT IS UNS AT 47

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 68

STEREO ATTRIBUTES: NONE

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@23 24

C~CF3
@25 26

C~OH
@27 28

C~Me
@29 30

C~OMe
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C~OEt
@33 34

C~Ak
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C~O~Ak
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@42 41 40

C~Ak~F
@43 44 45

C~Cy
@46 47

C~CN
48 49

C~Et
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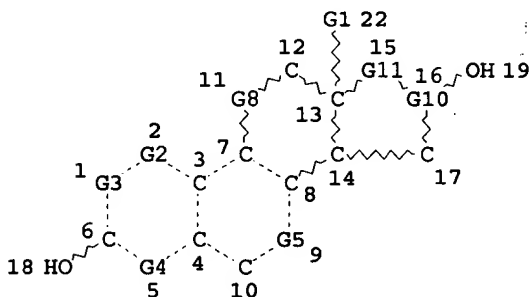
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C~CH2Cl
@55 56 57

C~G9
@58 59

C~S~Ak
@60 61 63

S @62



C~CH2 CN
@64 65 66

C~F
@67 68

VAR G1=ME/ET/CF3/20

VAR G2=CH/23/27/25/29/31/33

VAR G3=CH/23/27/35/37

VAR G4=CH/23/35/25/42/37

VAR G5=CH/23/35/43/37/46

VAR G8=CH2/CH/52/27/58/23/55/35/43/37/46

VAR G9=62/60

VAR G10=CH/35/43/25/42/64

VAR G11=CH2/CH/67/35/43

NODE ATTRIBUTES:

CONNECT IS E2 RC AT 61

CONNECT IS E1 RC AT 62

DEFAULT MLEVEL IS ATOM

GGCAT IS UNS AT 47

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 68

STEREO ATTRIBUTES: NONE

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L34 46181 SEA FILE=HCAPLUS ABB=ON PLU=ON STEROID?/SC,SX
L35 362 SEA FILE=HCAPLUS ABB=ON PLU=ON L31 AND L34
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L49 16 SEA FILE=HCAPLUS ABB=ON PLU=ON L46 AND L42
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L52 ANSWER 1 OF 24 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2000:552017 HCAPLUS

DOCUMENT NUMBER: 133:150782

TITLE: synthesis of 16-Hydroxyestratrienes as
selectively effective **estrogens**

INVENTOR(S): Kuenzer, Hermann; Knauthe, Rudolf; Lessl,
Monika; Fritzemeier, Karl-heinrich;
Hegele-Hartung, Christa; Boemer, Ulf; Mueller,
Gerd; Kosemund, Dirk

PATENT ASSIGNEE(S): Schering A.-G., Germany

SOURCE: Ger. Offen., 34 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent

LANGUAGE: German

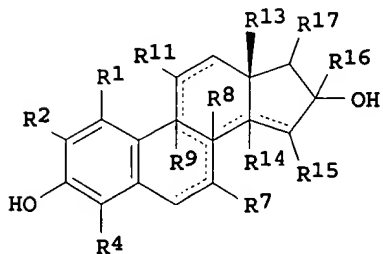
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 19906159	A1	20000810	DE 1999-19906159	1999 0209
CA 2359660	AA	20000817	CA 2000-2359660	2000 0209
WO 2000047603	A2	20000817	WO 2000-EP1073	2000 0209
WO 2000047603	A3	20010802		
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
AU 2000029095	A5	20000829	AU 2000-29095	

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EP 1144431	A2	20011017	EP 2000-907539	
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EP 1144431	B1	20051221		
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				0209

OTHER SOURCE(S): MARPAT 133:150782
GI



AB Synthesis of 16-Hydroxyestratrienes (I) [R1 = halogen, HO, Me, F3C, MeO, EtO, H; R2 = halogen, HO, (un)substituted alkoxy, H; R4 = halogen, fluoroalkyl, F3C, F5C2, (un)substituted alkoxy, H; R7 = halogen, (un)substituted alkyl, (un)substituted alkenyl, (un)substituted alkoxy, (un)substituted heteroaryl, (un)substituted aryl, H; R8 = H, fluoroalkyl, fluoroalkenyl, CN; R9 = H, Me, Et, F3C, F5C2; R11 = NO2O, HO, HS, halogen, chloromethyl, fluoroalkenyl, fluoroalkyl, (un)substituted alkoxy, (un)substituted alkylthio, (un)substituted aryl, (un)substituted heteroaryl, H; R13 = Me, Et, F3C, F5C2; R14 = (un)substituted alkenyl, (un)substituted alkyl, H; R15 = halogen, fluoroalkyl, fluoroalkenyl, =O, =S, SO, SO2, (un)substituted =NH; R14, R15 together = methylene; R16 = fluoroalkyl, fluoroalkenyl, F3C, F5C2, CN, H; R17 = fluoroalkyl, fluoroalkenyl, H, HO] as selectively effective estrogens is disclosed. Thus, 16 α -estradiol shows a 50% uterine stimulation at 30 ug in vivo testing.

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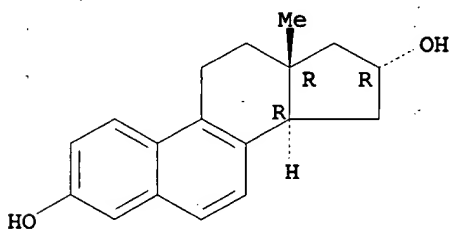
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 287723-82-4P 287723-83-5P 287723-84-6P
 287723-85-7P 287723-86-8P 287723-87-9P
 287723-88-0P 287723-89-1P 287723-90-4P
 287723-91-5P 287723-92-6P

RL: BAC (Biological activity or effector, except adverse); BSU
 (Biological study, unclassified); SPN (Synthetic preparation);
 THU (Therapeutic use); BIOL (Biological study); PREP
 (Preparation); USES (Uses)
 (synthesis of 16-Hydroxyestratrienes as selectively effective
 estrogens)

RN 109932-04-9 HCAPLUS

CN Estr-1,3,5(10),6,8-pentaene-3,16-diol, (16 α)- (9CI) (CA
 INDEX NAME)

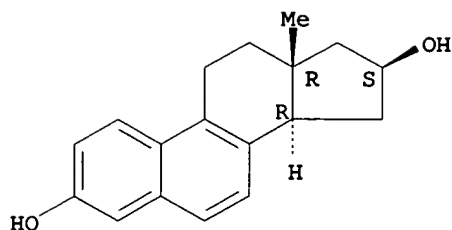
Absolute stereochemistry.



RN 110012-46-9 HCAPLUS

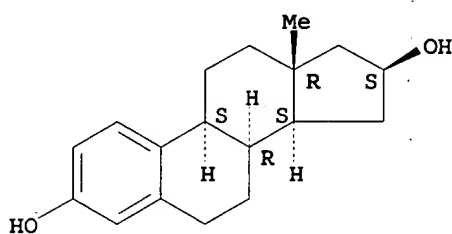
CN Estr-1,3,5(10),6,8-pentaene-3,16-diol, (16 β)- (9CI) (CA
 INDEX NAME)

Absolute stereochemistry.



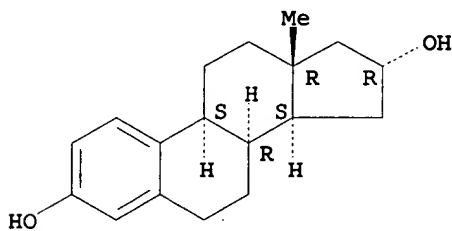
RN 287721-55-5 HCAPLUS
 CN Estra-1,3,5(10)-triene-3,16-diol, (8 α ,16 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



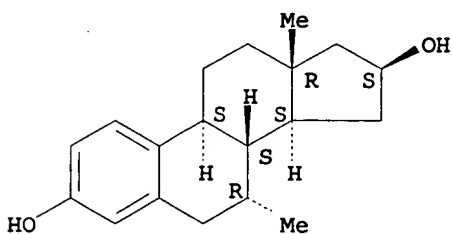
RN 287721-56-6 HCAPLUS
 CN Estra-1,3,5(10)-triene-3,16-diol, (8 α ,16 α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



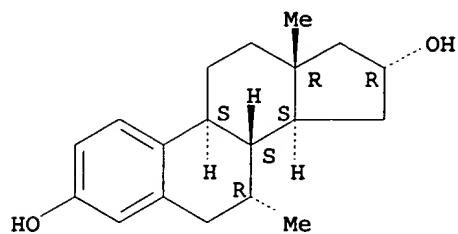
RN 287721-57-7 HCAPLUS
 CN Estra-1,3,5(10)-triene-3,16-diol, 7-methyl-, (7 α ,16 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



RN 287721-58-8 HCAPLUS
 CN Estra-1,3,5(10)-triene-3,16-diol, 7-methyl-, (7 α ,16 α)- (9CI) (CA INDEX NAME)

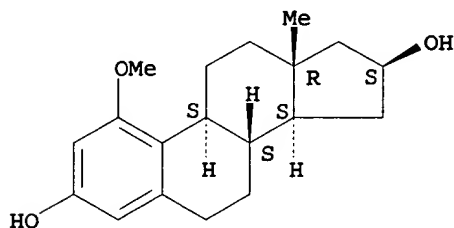
Absolute stereochemistry. Rotation (+).



RN 287721-59-9 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 1-methoxy-, (16β)- (9CI)
(CA INDEX NAME)

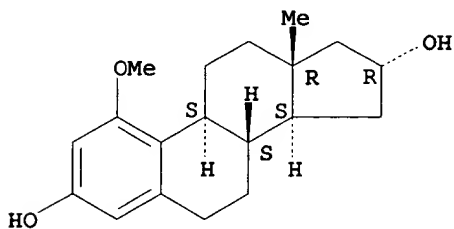
Absolute stereochemistry.



RN 287721-60-2 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 1-methoxy-, (16α)- (9CI)
(CA INDEX NAME)

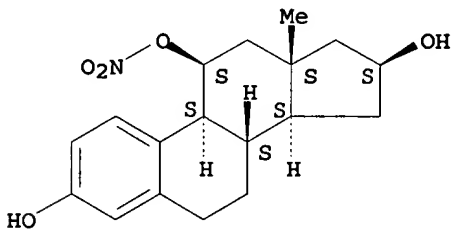
Absolute stereochemistry.



RN 287721-61-3 HCAPLUS

CN Estra-1,3,5(10)-triene-3,11,16-triol, 11-nitrate,
(11β,16β)- (9CI) (CA INDEX NAME)

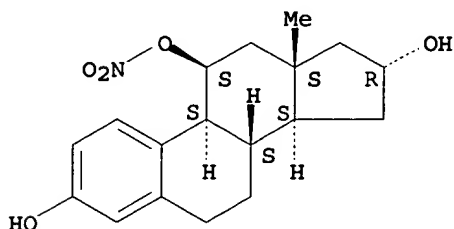
Absolute stereochemistry. Rotation (+).



RN 287721-62-4 HCAPLUS

CN Estra-1,3,5(10)-triene-3,11,16-triol, 11-nitrate,
(11 β ,16 α)- (9CI) (CA INDEX NAME)

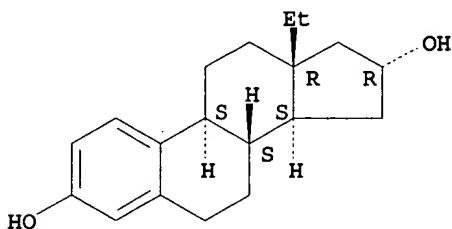
Absolute stereochemistry. Rotation (+).



RN 287721-63-5 HCAPLUS

CN Gona-1,3,5(10)-triene-3,16-diol, 13-ethyl-, (16 α)- (9CI)
(CA INDEX NAME)

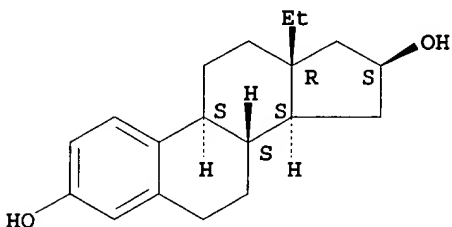
Absolute stereochemistry. Rotation (+).



RN 287721-64-6 HCAPLUS

CN Gona-1,3,5(10)-triene-3,16-diol, 13-ethyl-, (16 β)- (9CI) (CA
INDEX NAME)

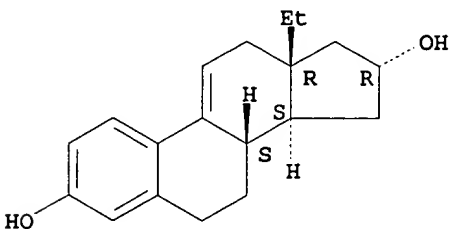
Absolute stereochemistry. Rotation (+).



RN 287721-65-7 HCAPLUS

CN Gona-1,3,5(10),9(11)-tetraene-3,16-diol, 13-ethyl-, (16 α)-
(9CI) (CA INDEX NAME)

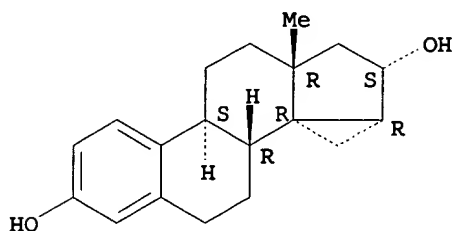
Absolute stereochemistry. Rotation (+).



RN 287721-66-8 HCAPLUS

CN Cycloprop[14,15]estra-1,3,5(10)-triene-3,16-diol, 3',15-dihydro-, (14R,15 β ,16 α)- (9CI) (CA INDEX NAME)

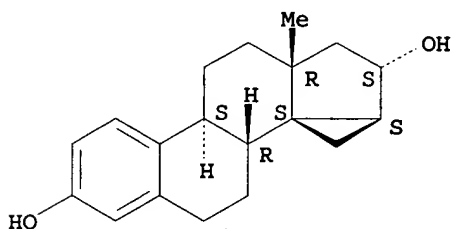
Absolute stereochemistry.



RN 287721-67-9 HCAPLUS

CN Cycloprop[14,15]estra-1,3,5(10)-triene-3,16-diol, 3',15-dihydro-, (14S,15 α ,16 α)- (9CI) (CA INDEX NAME)

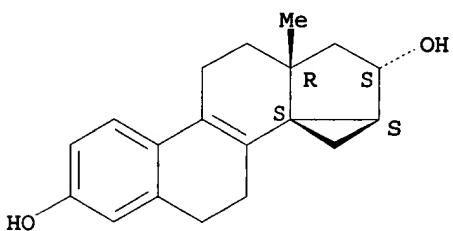
Absolute stereochemistry.



RN 287721-68-0 HCAPLUS

CN Cycloprop[14,15]estra-1,3,5(10),8-tetraene-3,16-diol, 3',15-dihydro-, (14S,15 α ,16 α)- (9CI) (CA INDEX NAME)

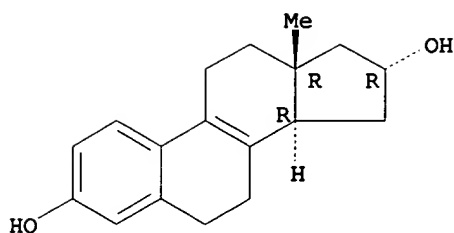
Absolute stereochemistry.



RN 287721-69-1 HCAPLUS

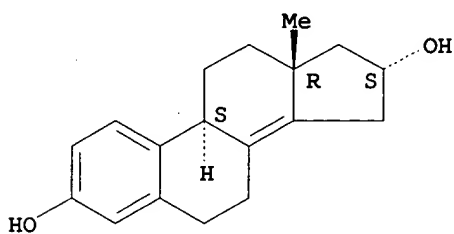
CN Estra-1,3,5(10),8-tetraene-3,16-diol, (16 α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



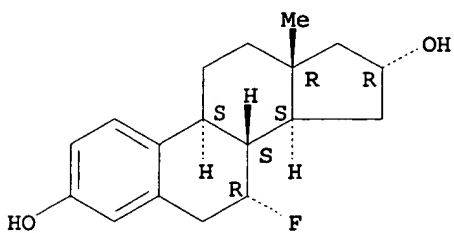
RN 287721-70-4 HCAPLUS
 CN Estra-1,3,5(10),8(14)-tetraene-3,16-diol, (16 α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



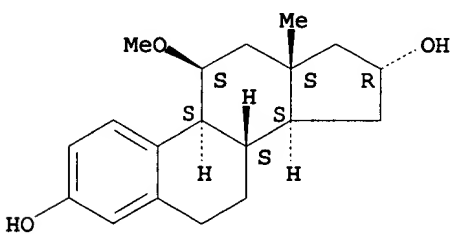
RN 287721-71-5 HCAPLUS
 CN Estra-1,3,5(10)-triene-3,16-diol, 7-fluoro-, (7 α ,16 α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



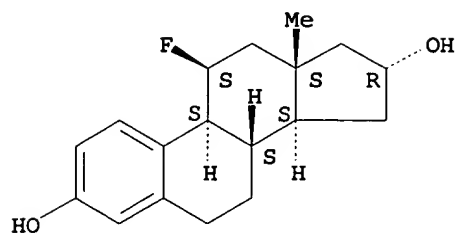
RN 287721-72-6 HCAPLUS
 CN Estra-1,3,5(10)-triene-3,16-diol, 11-methoxy-, (11 β ,16 α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



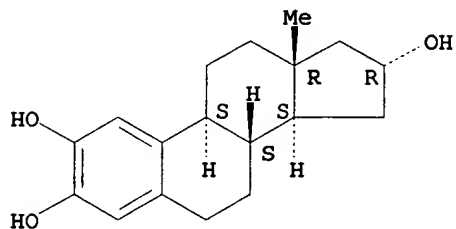
RN 287721-73-7 HCAPLUS
 CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-, (11 β ,16 α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



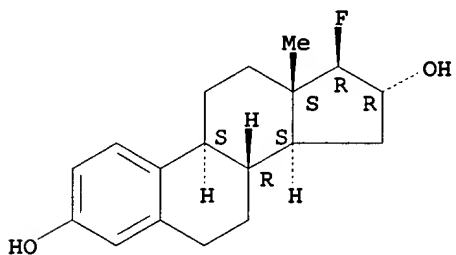
RN 287721-74-8 HCAPLUS
CN Estra-1,3,5(10)-triene-2,3,16-triol, (16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



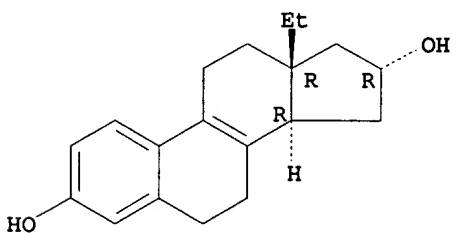
RN 287721-75-9 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 17-fluoro-, (16α,17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



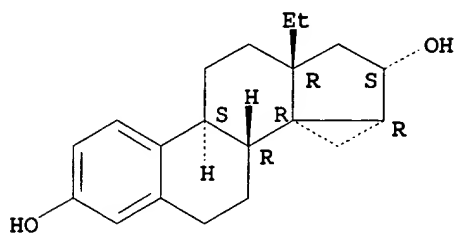
RN 287721-76-0 HCAPLUS
CN Gona-1,3,5(10),8-tetraene-3,16-diol, 13-ethyl-, (16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



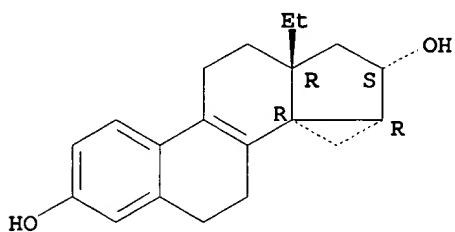
RN 287721-77-1 HCAPLUS
 CN Cyclopropa[14,15]gona-1,3,5(10)-triene-3,16-diol,
 13-ethyl-3',15-dihydro-, (14R,15 β ,16 α)- (9CI) (CA
 INDEX NAME)

Absolute stereochemistry.



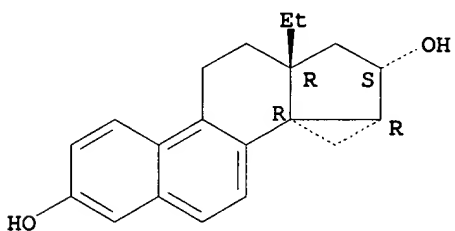
RN 287721-78-2 HCAPLUS
 CN Cyclopropa[14,15]gona-1,3,5(10),8-tetraene-3,16-diol,
 13-ethyl-3',15-dihydro-, (14R,15 β ,16 α)- (9CI) (CA
 INDEX NAME)

Absolute stereochemistry.



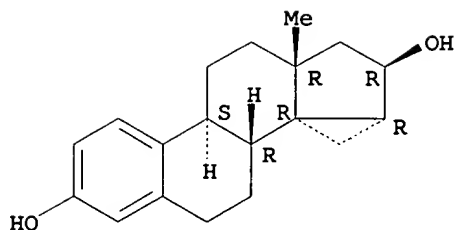
RN 287721-79-3 HCAPLUS
 CN Cyclopropa[14,15]gona-1,3,5,7,9-pentaene-3,16-diol,
 13-ethyl-3',15-dihydro-, (14R,15 β ,16 α)- (9CI) (CA
 INDEX NAME)

Absolute stereochemistry.



RN 287721-80-6 HCAPLUS
 CN Cycloprop[14,15]estra-1,3,5(10)-triene-3,16-diol, 3',15-dihydro-,
 (14R,15 β ,16 β)- (9CI) (CA INDEX NAME)

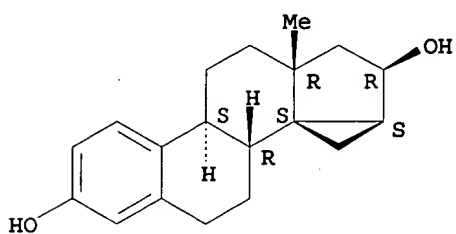
Absolute stereochemistry.



RN 287721-81-7 HCAPLUS

CN Cycloprop[14,15]estra-1,3,5(10)-triene-3,16-diol, 3',15-dihydro-, (14S,15 α ,16 β)- (9CI) (CA INDEX NAME)

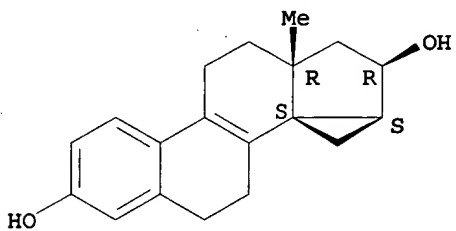
Absolute stereochemistry.



RN 287721-82-8 HCAPLUS

CN Cycloprop[14,15]estra-1,3,5(10),8-tetraene-3,16-diol, 3',15-dihydro-, (14S,15 α ,16 β)- (9CI) (CA INDEX NAME)

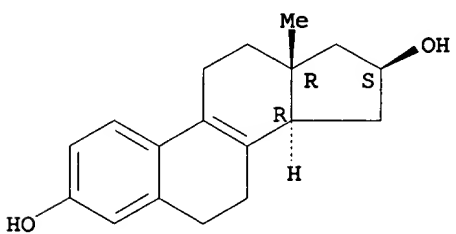
Absolute stereochemistry.



RN 287721-83-9 HCAPLUS

CN Estra-1,3,5(10),8-tetraene-3,16-diol, (16 β)- (9CI) (CA INDEX NAME)

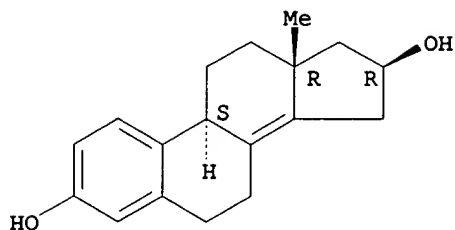
Absolute stereochemistry.



RN 287721-84-0 HCAPLUS

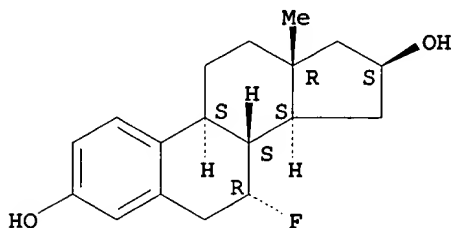
CN Estra-1,3,5(10),8(14)-tetraene-3,16-diol, (16 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



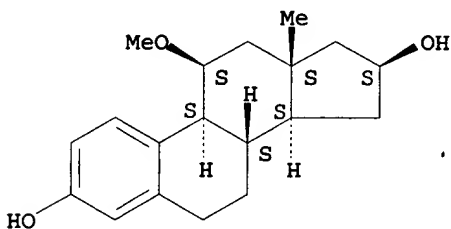
RN 287721-85-1 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 7-fluoro-, (7 α ,16 β)-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.



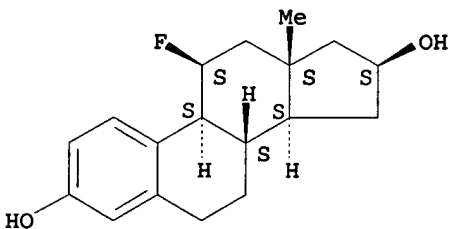
RN 287721-86-2 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 11-methoxy-,
(11 β ,16 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 287721-87-3 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-, (11 β ,16 β)-
(9CI) (CA INDEX NAME)

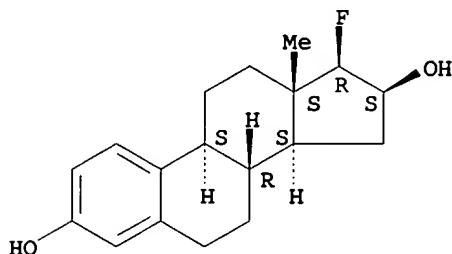
Absolute stereochemistry.



RN 287721-88-4 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 17-fluoro-, (16 β ,17 β)-
(9CI) (CA INDEX NAME)

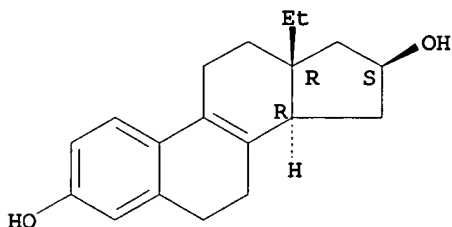
Absolute stereochemistry.



RN 287721-89-5 HCAPLUS

CN Gona-1,3,5(10),8-tetraene-3,16-diol, 13-ethyl-, (16 β)- (9CI)
(CA INDEX NAME)

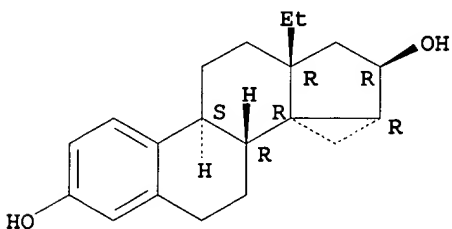
Absolute stereochemistry.



RN 287721-90-8 HCAPLUS

CN Cyclopropa[14,15]gona-1,3,5(10)-triene-3,16-diol,
13-ethyl-3',15-dihydro-, (14R,15 β ,16 β)- (9CI) (CA INDEX
NAME)

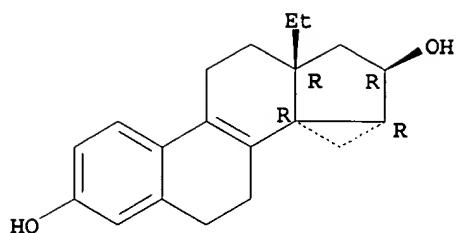
Absolute stereochemistry.



RN 287721-91-9 HCAPLUS

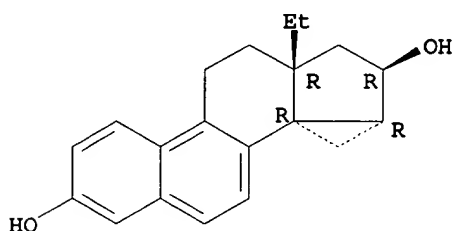
CN Cyclopropa[14,15]gona-1,3,5(10),8-tetraene-3,16-diol,
13-ethyl-3',15-dihydro-, (14R,15 β ,16 β)- (9CI) (CA INDEX
NAME)

Absolute stereochemistry.



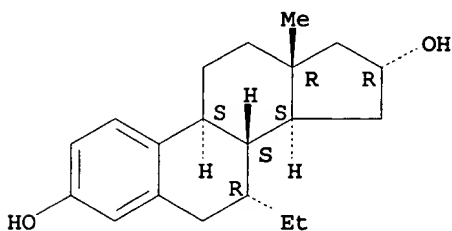
RN 287721-92-0 HCAPLUS
 CN Cyclopropa[14,15]gona-1,3,5,7,9-pentaene-3,16-diol,
 13-ethyl-3',15-dihydro-, (14R,15β,16β)- (9CI) (CA INDEX
 NAME)

Absolute stereochemistry.



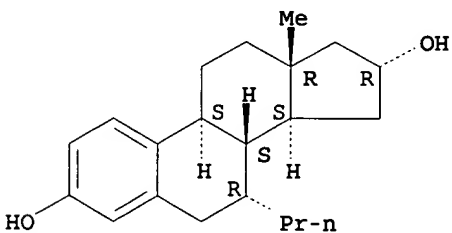
RN 287721-93-1 HCAPLUS
 CN Estra-1,3,5(10)-triene-3,16-diol, 7-ethyl-, (7α,16α)-
 (9CI) (CA INDEX NAME)

Absolute stereochemistry.



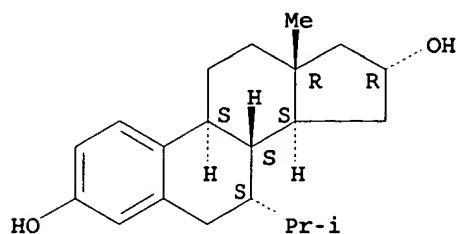
RN 287721-94-2 HCAPLUS
 CN Estra-1,3,5(10)-triene-3,16-diol, 7-propyl-, (7α,16α)-
 (9CI) (CA INDEX NAME)

Absolute stereochemistry.



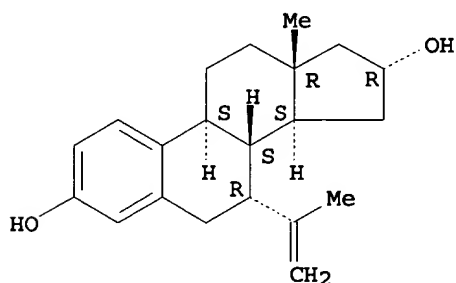
RN 287721-95-3 HCAPLUS
 CN Estra-1,3,5(10)-triene-3,16-diol, 7-(1-methylethyl)-,

Absolute stereochemistry.



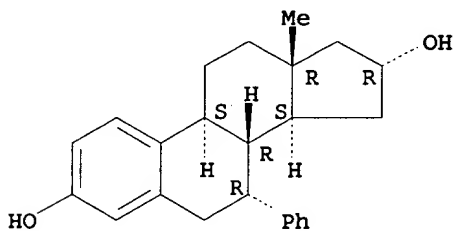
CN Estr-1,3,5(10)-triene-3,16-diol, 7-(1-methylethenyl)-,
(7 α ,16 α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



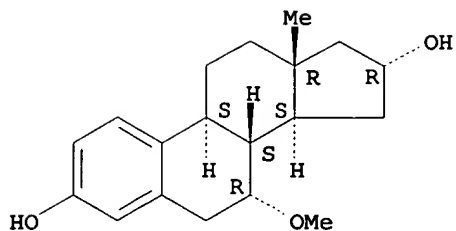
CN Estr-1,3,5(10)-triene-3,16-diol, 7-phenyl-, (7 α ,16 α)-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.



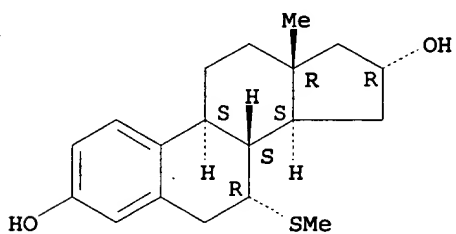
CN Estr-1,3,5(10)-triene-3,16-diol, 7-methoxy-, (7 α ,16 α)-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.



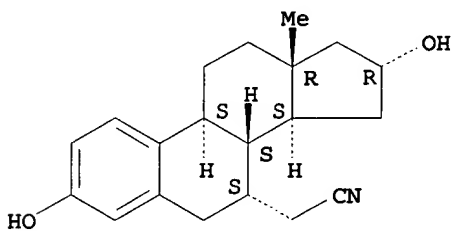
RN 287721-99-7 HCAPLUS
 CN Estradiol, 7-(methylthio)-, (7 α ,16 α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



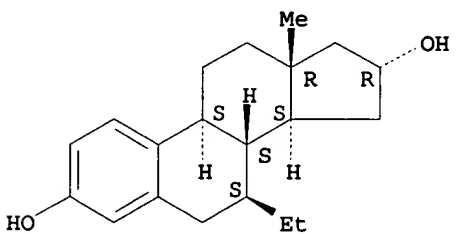
RN 287722-00-3 HCAPLUS
 CN Estradiol, 7-(methylthio)-, (7 α ,16 α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



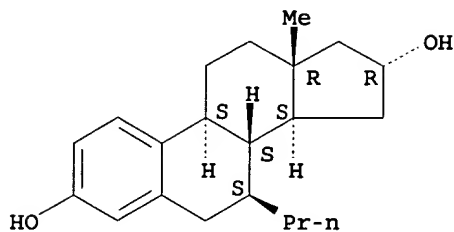
RN 287722-01-4 HCAPLUS
 CN Estradiol, 7-(methylthio)-, (7 α ,16 α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 287722-02-5 HCAPLUS
 CN Estradiol, 7-(methylthio)-, (7 α ,16 α)- (9CI) (CA INDEX NAME)

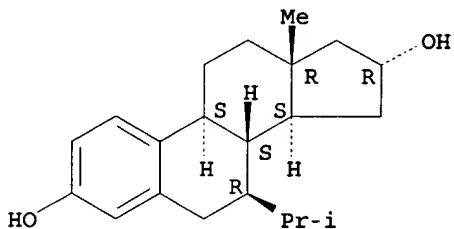
Absolute stereochemistry.



RN 287722-03-6 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 7-(1-methylethyl)-,
(7β,16α)- (9CI) (CA INDEX NAME)

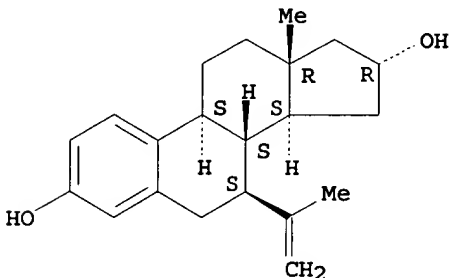
Absolute stereochemistry.



RN 287722-04-7 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 7-(1-methylethenyl)-,
(7β,16α)- (9CI) (CA INDEX NAME)

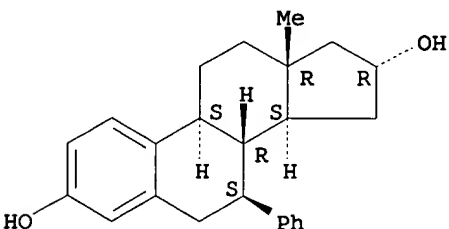
Absolute stereochemistry.



RN 287722-05-8 HCAPLUS

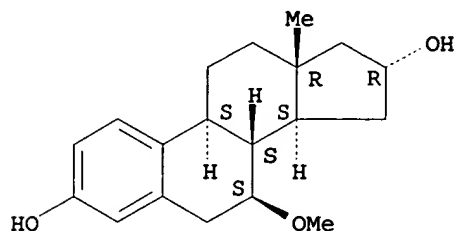
CN Estra-1,3,5(10)-triene-3,16-diol, 7-phenyl-, (7β,16α)-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.



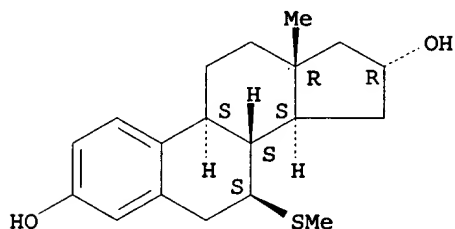
RN 287722-06-9 HCAPLUS
 CN Estra-1,3,5(10)-triene-3,16-diol, 7-methoxy-, (7 β ,16 α)-
 (9CI) (CA INDEX NAME)

Absolute stereochemistry.



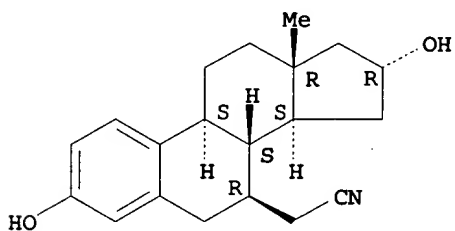
RN 287722-07-0 HCAPLUS
 CN Estra-1,3,5(10)-triene-3,16-diol, 7-(methylthio)-,
 (7 β ,16 α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



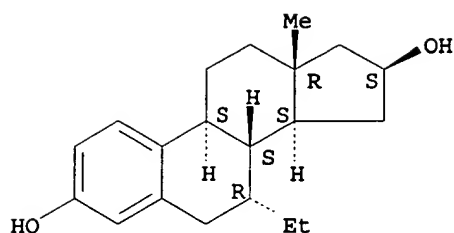
RN 287722-08-1 HCAPLUS
 CN Estra-1,3,5(10)-triene-7-acetonitrile, 3,16-dihydroxy-,
 (7 β ,16 α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



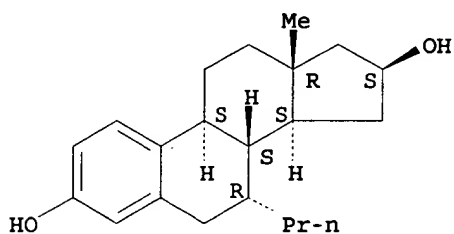
RN 287722-09-2 HCAPLUS
 CN Estra-1,3,5(10)-triene-3,16-diol, 7-ethyl-, (7 α ,16 β)-
 (9CI) (CA INDEX NAME)

Absolute stereochemistry.



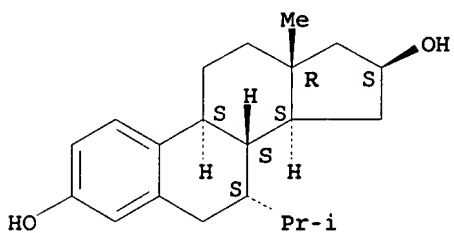
RN 287722-10-5 HCAPLUS
 CN Estra-1,3,5(10)-triene-3,16-diol, 7-propyl-, (7 α ,16 β)-
 (9CI) (CA INDEX NAME)

Absolute stereochemistry.



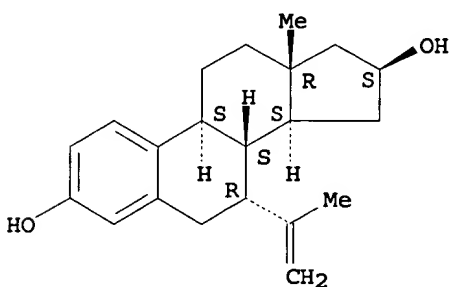
RN 287722-11-6 HCAPLUS
 CN Estra-1,3,5(10)-triene-3,16-diol, 7-(1-methylethyl)-,
 (7 α ,16 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 287722-12-7 HCAPLUS
 CN Estra-1,3,5(10)-triene-3,16-diol, 7-(1-methylethenyl)-,
 (7 α ,16 β)- (9CI) (CA INDEX NAME)

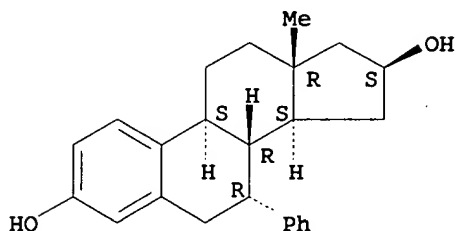
Absolute stereochemistry.



RN 287722-13-8 HCAPLUS

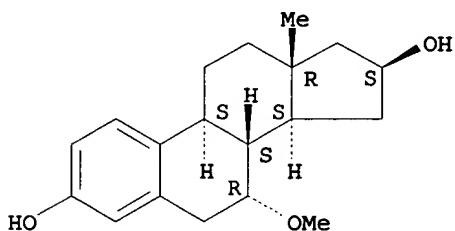
CN Estr-1,3,5(10)-triene-3,16-diol, 7-phenyl-, (7 α ,16 β)-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.



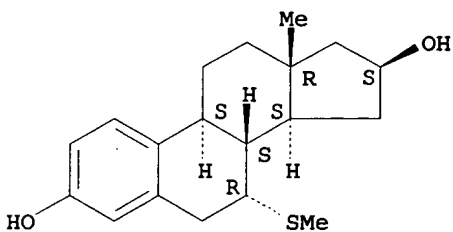
RN 287722-14-9 HCAPLUS
CN Estr-1,3,5(10)-triene-3,16-diol, 7-methoxy-, (7 α ,16 β)-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.



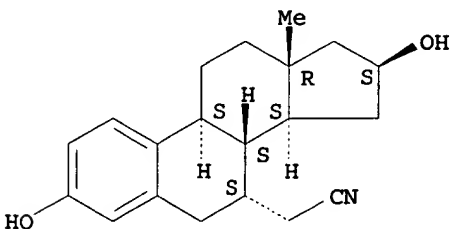
RN 287722-15-0 HCAPLUS
CN Estr-1,3,5(10)-triene-3,16-diol, 7-(methylthio)-,
(7 α ,16 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 287722-16-1 HCAPLUS
CN Estr-1,3,5(10)-triene-7-acetonitrile, 3,16-dihydroxy-,
(7 α ,16 β)- (9CI) (CA INDEX NAME)

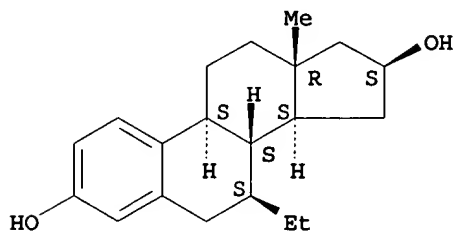
Absolute stereochemistry.



RN 287722-17-2 HCAPLUS

CN Estr-1,3,5(10)-triene-3,16-diol, 7-ethyl-, (7 β ,16 β)-
(9CI) (CA INDEX NAME)

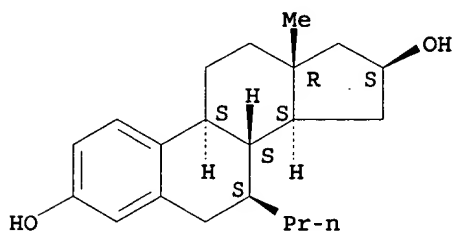
Absolute stereochemistry.



RN 287722-18-3 HCAPLUS

CN Estr-1,3,5(10)-triene-3,16-diol, 7-propyl-, (7 β ,16 β)-
(9CI) (CA INDEX NAME)

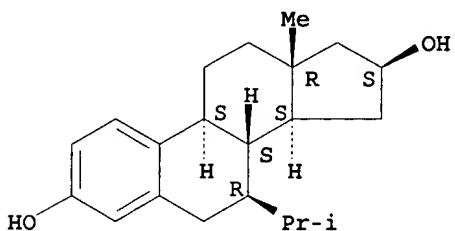
Absolute stereochemistry.



RN 287722-19-4 HCAPLUS

CN Estr-1,3,5(10)-triene-3,16-diol, 7-(1-methylethyl)-,
(7 β ,16 β)- (9CI) (CA INDEX NAME)

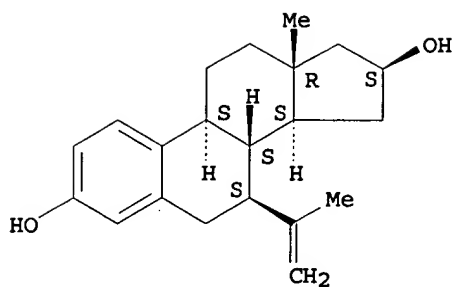
Absolute stereochemistry.



RN 287722-20-7 HCAPLUS

CN Estr-1,3,5(10)-triene-3,16-diol, 7-(1-methylethenyl)-,
(7 β ,16 β)- (9CI) (CA INDEX NAME)

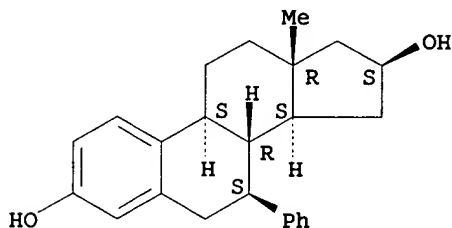
Absolute stereochemistry.



RN 287722-21-8 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 7-phenyl-, (7β,16β)-(9CI) (CA INDEX NAME)

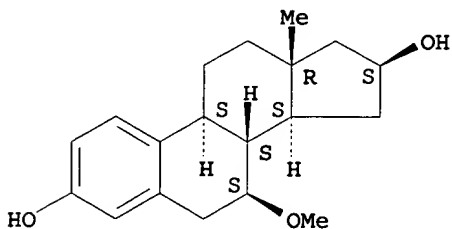
Absolute stereochemistry.



RN 287722-22-9 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 7-methoxy-, (7β,16β)-(9CI) (CA INDEX NAME)

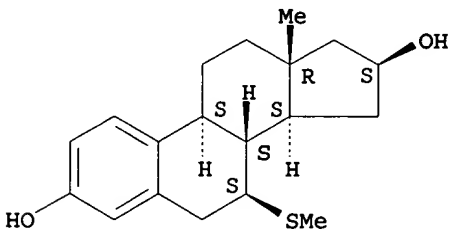
Absolute stereochemistry.



RN 287722-23-0 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 7-(methylthio)-, (7β,16β)-(9CI) (CA INDEX NAME)

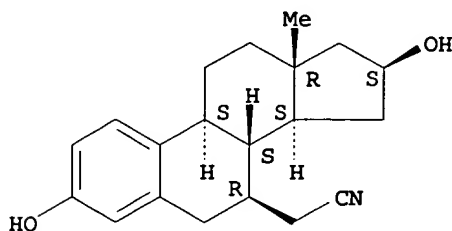
Absolute stereochemistry.



RN 287722-24-1 HCAPLUS

CN Estra-1,3,5(10)-triene-7-acetonitrile, 3,16-dihydroxy-,
(7 β ,16 β)- (9CI) (CA INDEX NAME)

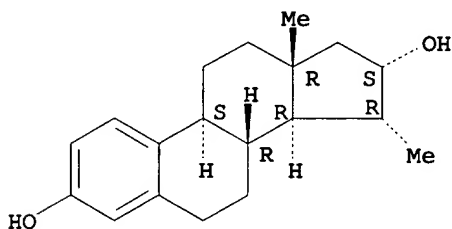
Absolute stereochemistry.



RN 287722-25-2 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 15-methyl-,
(15 α ,16 α)- (9CI) (CA INDEX NAME)

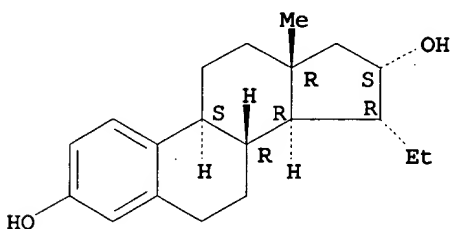
Absolute stereochemistry.



RN 287722-26-3 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 15-ethyl-, (15 α ,16 α)-
(9CI) (CA INDEX NAME)

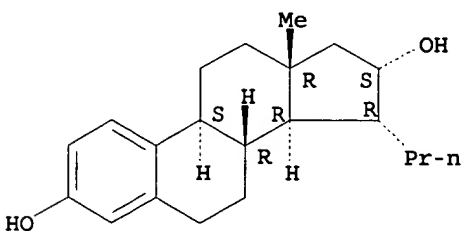
Absolute stereochemistry.



RN 287722-27-4 HCAPLUS

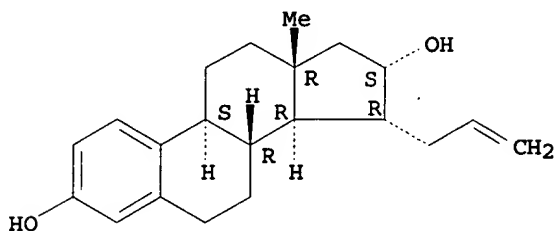
CN Estra-1,3,5(10)-triene-3,16-diol, 15-propyl-,
(15 α ,16 α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



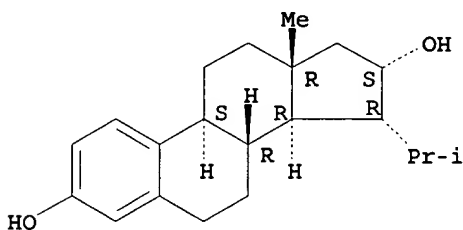
RN 287722-28-5 HCAPLUS
CN Estr-1,3,5(10)-triene-3,16-diol, 15-(2-propenyl)-,
(15 α ,16 α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



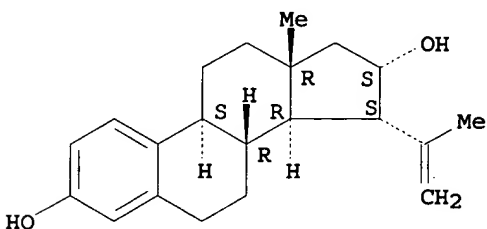
RN 287722-29-6 HCAPLUS
CN Estr-1,3,5(10)-triene-3,16-diol, 15-(1-methylethyl)-,
(15 α ,16 α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



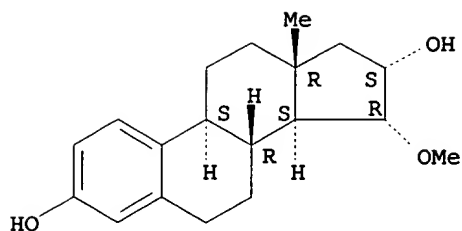
RN 287722-30-9 HCAPLUS
CN Estr-1,3,5(10)-triene-3,16-diol, 15-(1-methylethenyl)-,
(15 α ,16 α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



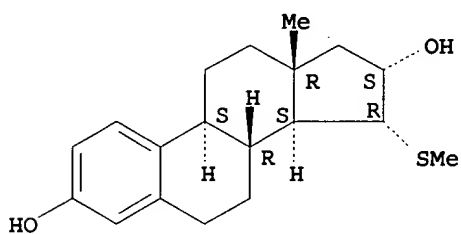
RN 287722-31-0 HCAPLUS
CN Estr-1,3,5(10)-triene-3,16-diol, 15-methoxy-,
(15 α ,16 α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



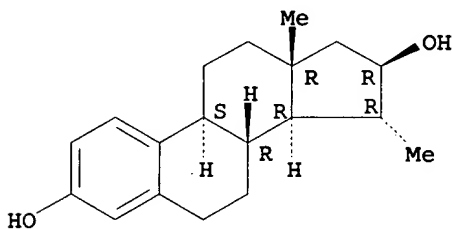
RN 287722-32-1 HCAPLUS
 CN Estradiol 15-methylthio ether, (15 α ,16 α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



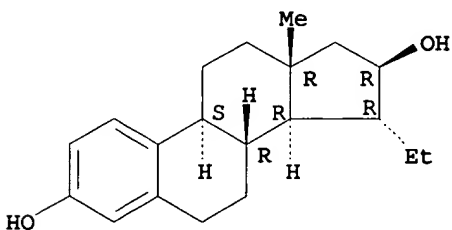
RN 287722-33-2 HCAPLUS
 CN Estradiol 15-methyl ether, (15 α ,16 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



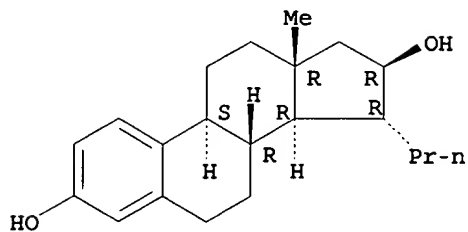
RN 287722-34-3 HCAPLUS
 CN Estradiol 15-ethyl ether, (15 α ,16 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



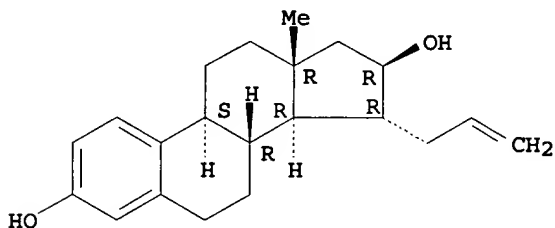
RN 287722-35-4 HCAPLUS
 CN Estradiol 15-propyl ether, (15 α ,16 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



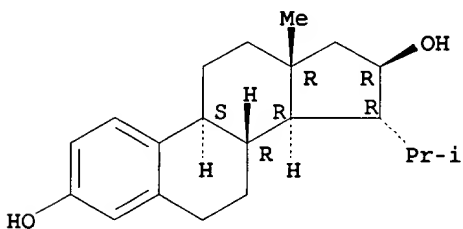
RN 287722-36-5 HCAPLUS
 CN Estradiol, 15-(2-propenyl)-,
 (15 α ,16 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



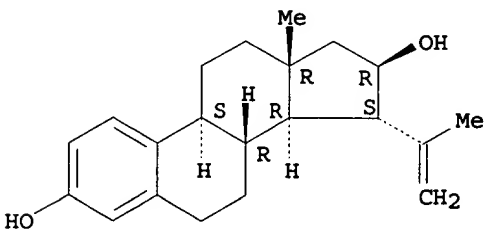
RN 287722-37-6 HCAPLUS
 CN Estradiol, 15-(1-methylethyl)-,
 (15 α ,16 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 287722-38-7 HCAPLUS
 CN Estradiol, 15-(1-methylethenyl)-,
 (15 α ,16 β)- (9CI) (CA INDEX NAME)

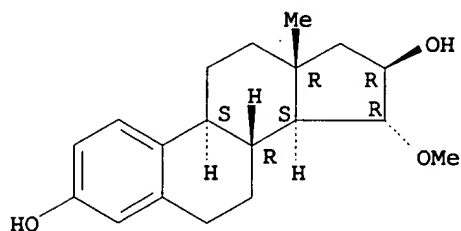
Absolute stereochemistry.



RN 287722-39-8 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 15-methoxy-,
(15 α ,16 β)- (9CI) (CA INDEX NAME)

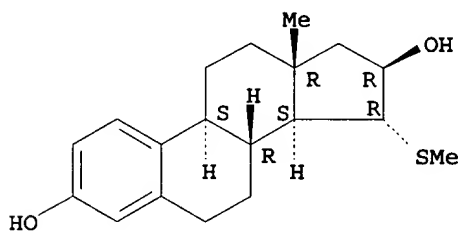
Absolute stereochemistry.



RN 287722-40-1 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 15-(methylthio)-,
(15 α ,16 β)- (9CI) (CA INDEX NAME)

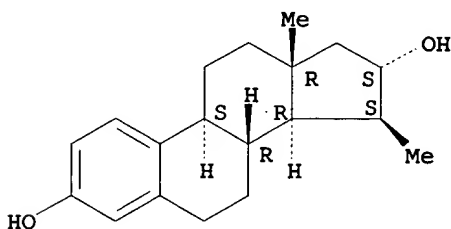
Absolute stereochemistry.



RN 287722-41-2 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 15-methyl-, (15 β ,16 α)-
(9CI) (CA INDEX NAME)

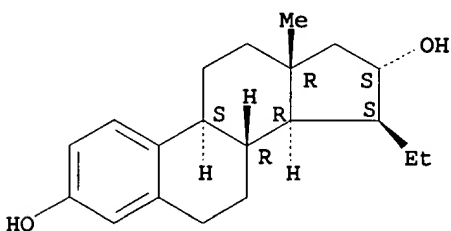
Absolute stereochemistry.



RN 287722-42-3 HCAPLUS

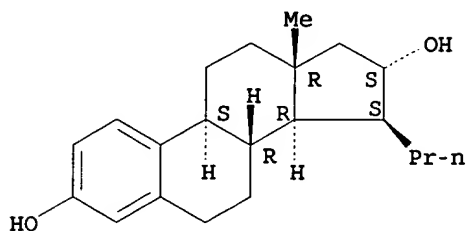
CN Estra-1,3,5(10)-triene-3,16-diol, 15-ethyl-, (15 β ,16 α)-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.



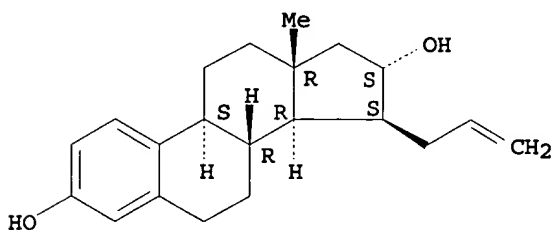
RN 287722-43-4 HCAPLUS
 CN Estra-1,3,5(10)-triene-3,16-diol, 15-propyl-, (15 β ,16 α)-
 (9CI) (CA INDEX NAME)

Absolute stereochemistry.



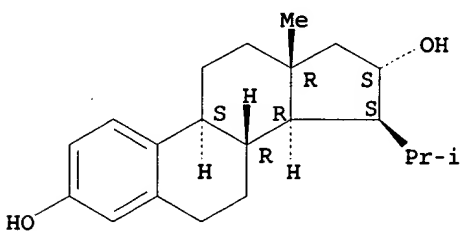
RN 287722-44-5 HCAPLUS
 CN Estra-1,3,5(10)-triene-3,16-diol, 15-(2-propenyl)-,
 (15 β ,16 α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



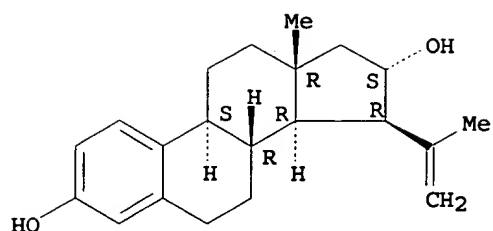
RN 287722-45-6 HCAPLUS
 CN Estra-1,3,5(10)-triene-3,16-diol, 15-(1-methylethyl)-,
 (15 β ,16 α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



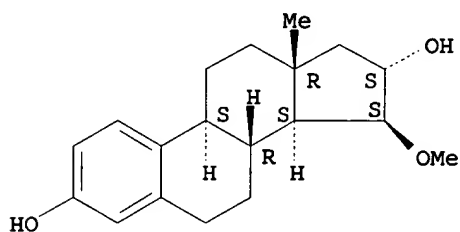
RN 287722-46-7 HCAPLUS
 CN Estra-1,3,5(10)-triene-3,16-diol, 15-(1-methylethenyl)-,
 (15 β ,16 α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



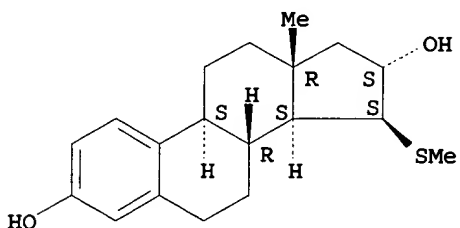
RN 287722-47-8 HCAPLUS
 CN Estra-1,3,5(10)-triene-3,16-diol, 15-methoxy-,
 (15 β ,16 α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



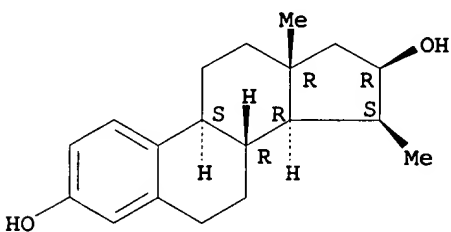
RN 287722-48-9 HCAPLUS
 CN Estra-1,3,5(10)-triene-3,16-diol, 15-(methylthio)-,
 (15 β ,16 α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



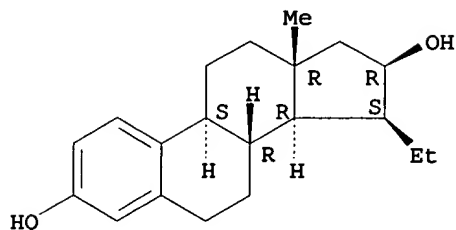
RN 287722-49-0 HCAPLUS
 CN Estra-1,3,5(10)-triene-3,16-diol, 15-methyl-, (15 β ,16 β)-
 (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 287722-50-3 HCAPLUS
 CN Estra-1,3,5(10)-triene-3,16-diol, 15-ethyl-, (15 β ,16 β)-
 (9CI) (CA INDEX NAME)

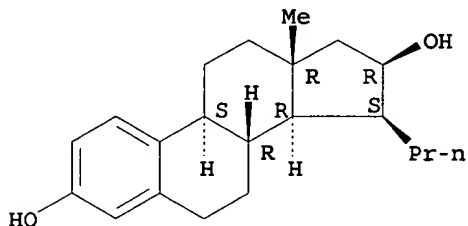
Absolute stereochemistry.



RN 287722-51-4 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 15-propyl-, (15 β ,16 β)-
(9CI) (CA INDEX NAME)

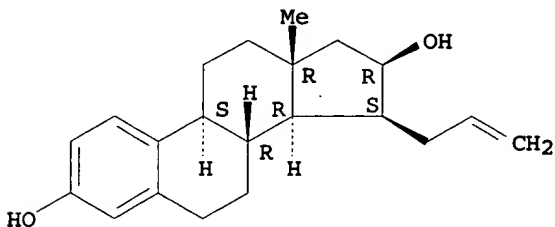
Absolute stereochemistry.



RN 287722-52-5 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 15-(2-propenyl)-,
(15 β ,16 β)- (9CI) (CA INDEX NAME)

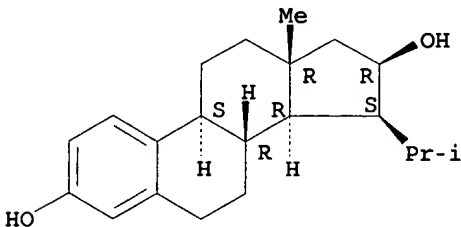
Absolute stereochemistry.



RN 287722-53-6 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 15-(1-methylethyl)-,
(15 β ,16 β)- (9CI) (CA INDEX NAME)

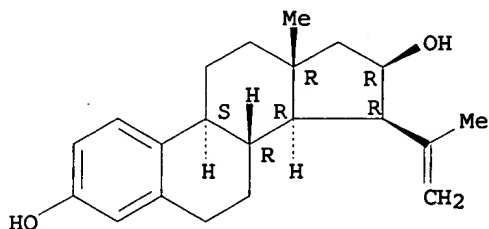
Absolute stereochemistry.



RN 287722-54-7 HCAPLUS

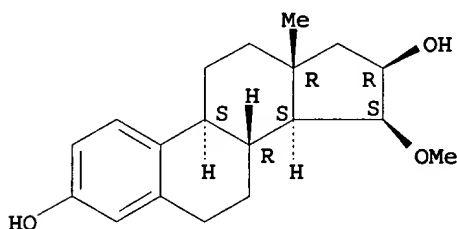
CN Estra-1,3,5(10)-triene-3,16-diol, 15-(1-methylethenyl)-,
(15 β ,16 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



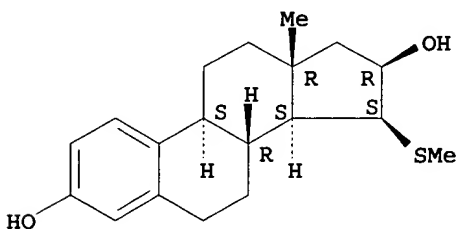
RN 287722-55-8 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 15-methoxy-,
(15 β ,16 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



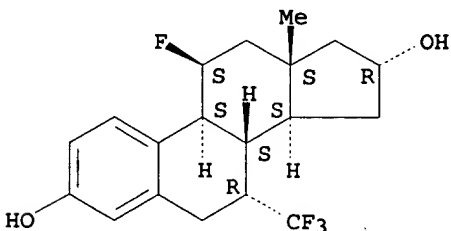
RN 287722-56-9 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 15-(methylthio)-,
(15 β ,16 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



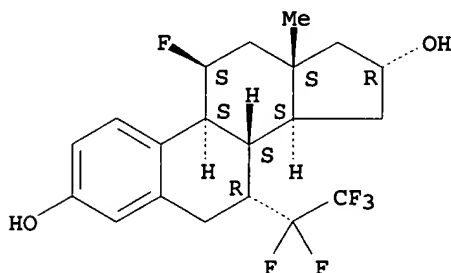
RN 287722-57-0 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-7-(trifluoromethyl)-,
(7 α ,11 β ,16 α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



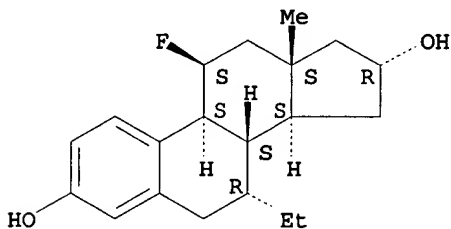
RN 287722-58-1 HCAPLUS
 CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-7-(pentafluoroethyl)-,
 (7 α ,11 β ,16 α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



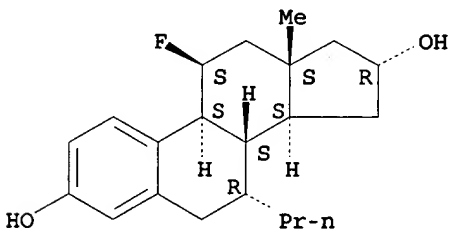
RN 287722-59-2 HCAPLUS
 CN Estra-1,3,5(10)-triene-3,16-diol, 7-ethyl-11-fluoro-,
 (7 α ,11 β ,16 α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



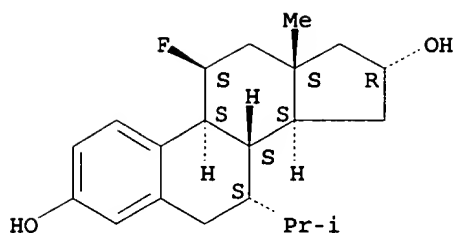
RN 287722-60-5 HCAPLUS
 CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-7-propyl-,
 (7 α ,11 β ,16 α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 287722-61-6 HCAPLUS
 CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-7-(1-methylethyl)-,
 (7 α ,11 β ,16 α)- (9CI) (CA INDEX NAME)

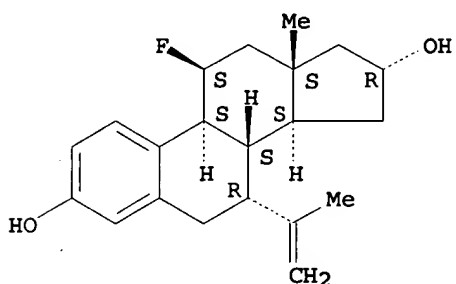
Absolute stereochemistry.



RN 287722-62-7 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-7-(1-methylethenyl)-,
(7 α ,11 β ,16 α)- (9CI) (CA INDEX NAME)

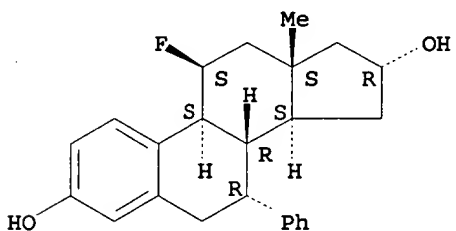
Absolute stereochemistry.



RN 287722-63-8 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-7-phenyl-,
(7 α ,11 β ,16 α)- (9CI) (CA INDEX NAME)

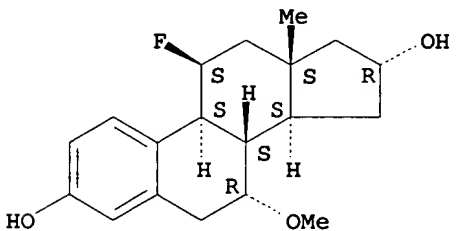
Absolute stereochemistry.



RN 287722-64-9 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-7-methoxy-,
(7 α ,11 β ,16 α)- (9CI) (CA INDEX NAME)

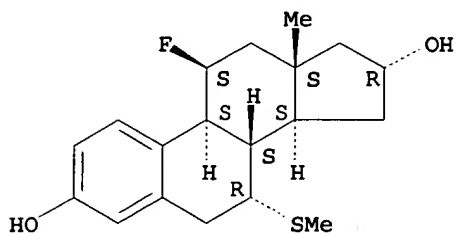
Absolute stereochemistry.



RN 287722-65-0 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-7-(methylthio)-,
(7 α ,11 β ,16 α)- (9CI) (CA INDEX NAME)

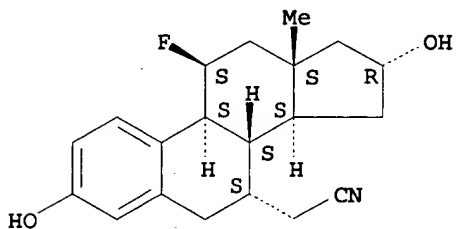
Absolute stereochemistry.



RN 287722-66-1 HCAPLUS

CN Estra-1,3,5(10)-triene-7-acetonitrile, 11-fluoro-3,16-dihydroxy-,
(7 α ,11 β ,16 α)- (9CI) (CA INDEX NAME)

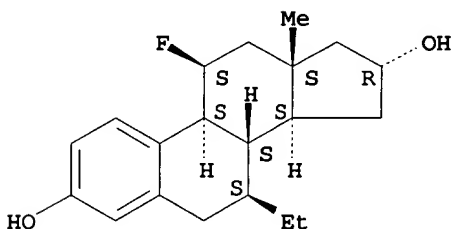
Absolute stereochemistry.



RN 287722-67-2 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 7-ethyl-11-fluoro-,
(7 β ,11 β ,16 α)- (9CI) (CA INDEX NAME)

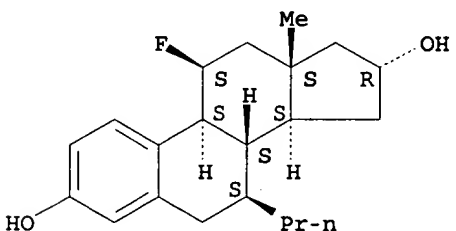
Absolute stereochemistry.



RN 287722-68-3 HCAPLUS

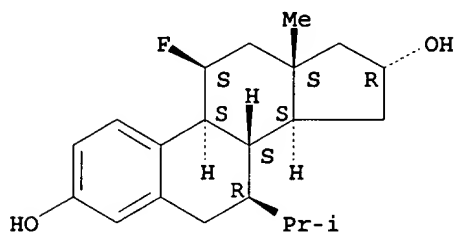
CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-7-propyl-,
(7 β ,11 β ,16 α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



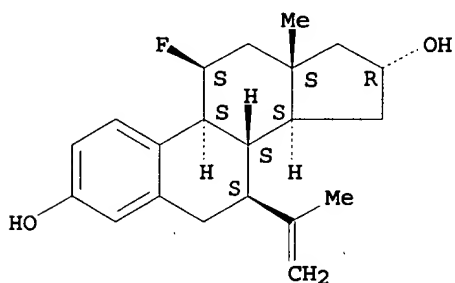
RN 287722-69-4 HCAPLUS
 CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-7-(1-methylethyl)-,
 (7 β ,11 β ,16 α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



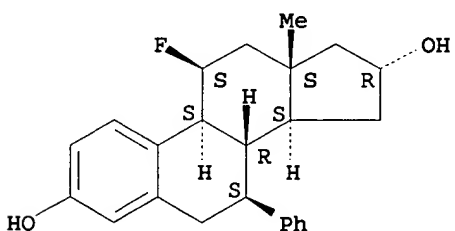
RN 287722-70-7 HCAPLUS
 CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-7-(1-methylethenyl)-,
 (7 β ,11 β ,16 α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



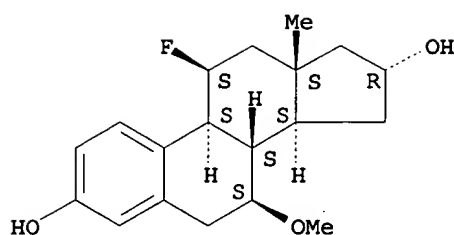
RN 287722-71-8 HCAPLUS
 CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-7-phenyl-,
 (7 β ,11 β ,16 α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 287722-72-9 HCAPLUS
 CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-7-methoxy-,
 (7 β ,11 β ,16 α)- (9CI) (CA INDEX NAME)

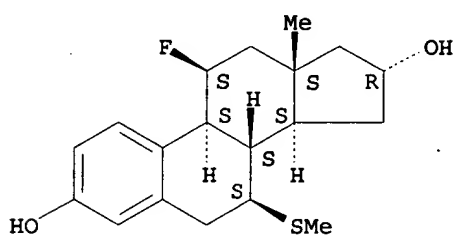
Absolute stereochemistry.



RN 287722-73-0 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-7-(methylthio)-,
(7 β ,11 β ,16 α)- (9CI) (CA INDEX NAME)

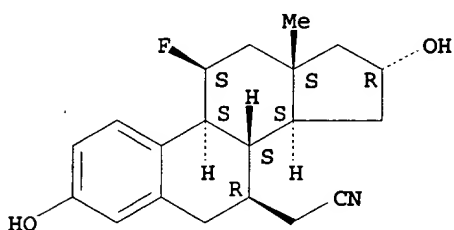
Absolute stereochemistry.



RN 287722-74-1 HCAPLUS

CN Estra-1,3,5(10)-triene-7-acetonitrile, 11-fluoro-3,16-dihydroxy-,
(7 β ,11 β ,16 α)- (9CI) (CA INDEX NAME)

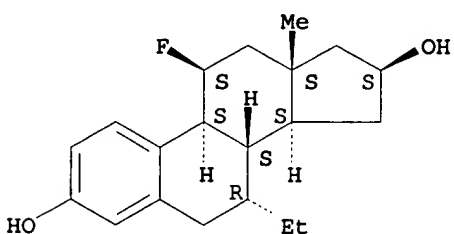
Absolute stereochemistry.



RN 287722-75-2 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 7-ethyl-11-fluoro-,
(7 α ,11 β ,16 β)- (9CI) (CA INDEX NAME)

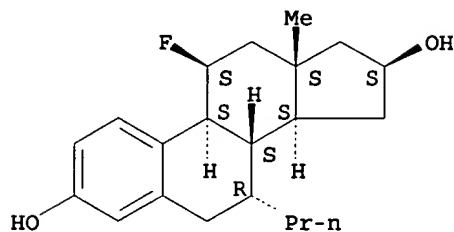
Absolute stereochemistry.



RN 287722-76-3 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-7-propyl-,
(7 α ,11 β ,16 β)- (9CI) (CA INDEX NAME)

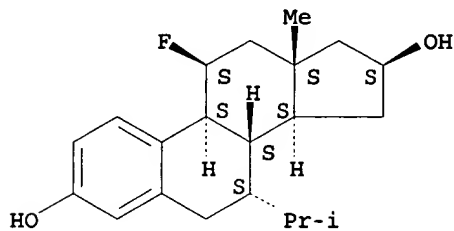
Absolute stereochemistry.



RN 287722-77-4 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-7-(1-methylethyl)-,
(7 α ,11 β ,16 β)- (9CI) (CA INDEX NAME)

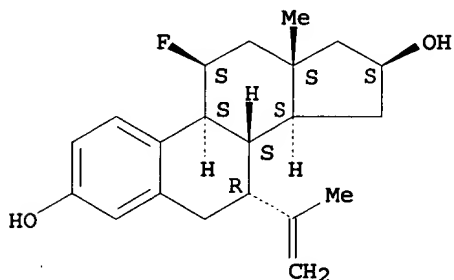
Absolute stereochemistry.



RN 287722-78-5 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-7-(1-methylethenyl)-,
(7 α ,11 β ,16 β)- (9CI) (CA INDEX NAME)

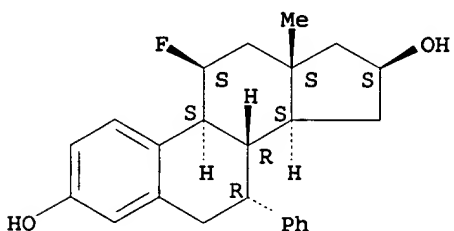
Absolute stereochemistry.



RN 287722-79-6 HCAPLUS

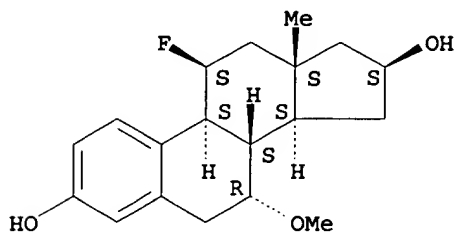
CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-7-phenyl-,
(7 α ,11 β ,16 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



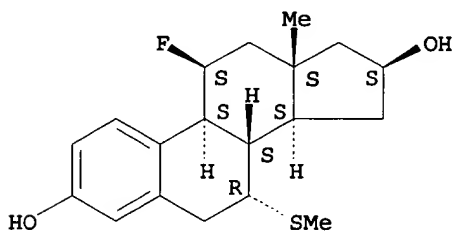
RN 287722-80-9 HCAPLUS
 CN Estr-1,3,5(10)-triene-3,16-diol, 11-fluoro-7-methoxy-,
 (7 α ,11 β ,16 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



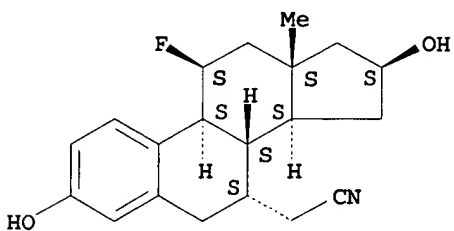
RN 287722-81-0 HCAPLUS
 CN Estr-1,3,5(10)-triene-3,16-diol, 11-fluoro-7-(methylthio)-,
 (7 α ,11 β ,16 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



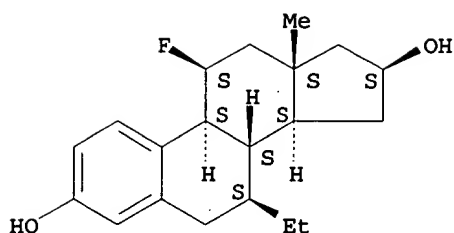
RN 287722-82-1 HCAPLUS
 CN Estr-1,3,5(10)-triene-7-acetonitrile, 11-fluoro-3,16-dihydroxy-,
 (7 α ,11 β ,16 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 287722-83-2 HCAPLUS
 CN Estr-1,3,5(10)-triene-3,16-diol, 7-ethyl-11-fluoro-,
 (7 β ,11 β ,16 β)- (9CI) (CA INDEX NAME)

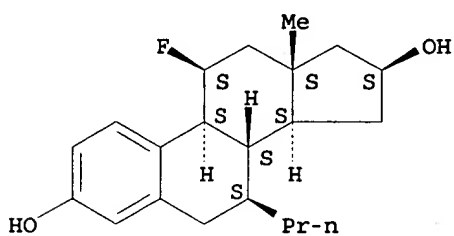
Absolute stereochemistry.



RN 287722-84-3 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-7-propyl-,
(7 β ,11 β ,16 β)- (9CI) (CA INDEX NAME)

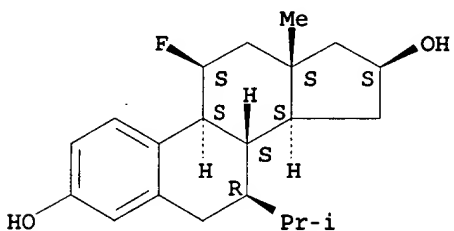
Absolute stereochemistry.



RN 287722-85-4 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-7-(1-methylethyl)-,
(7 β ,11 β ,16 β)- (9CI) (CA INDEX NAME)

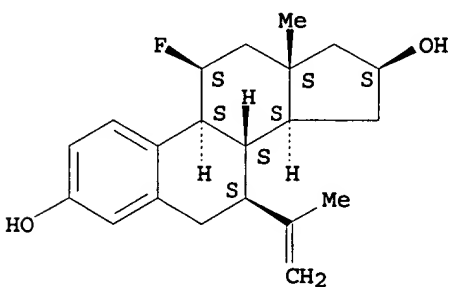
Absolute stereochemistry.



RN 287722-86-5 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-7-(1-methylethenyl)-,
(7 β ,11 β ,16 β)- (9CI) (CA INDEX NAME)

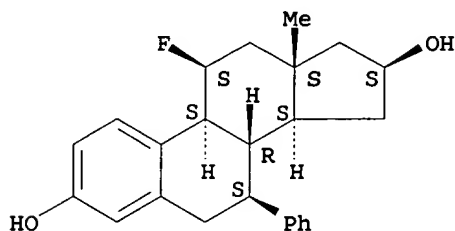
Absolute stereochemistry.



RN 287722-87-6 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-7-phenyl-,
(7 β ,11 β ,16 β)- (9CI) (CA INDEX NAME)

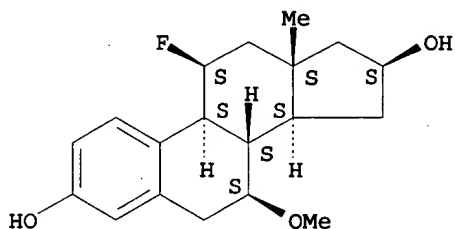
Absolute stereochemistry.



RN 287722-88-7 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-7-methoxy-,
(7 β ,11 β ,16 β)- (9CI) (CA INDEX NAME)

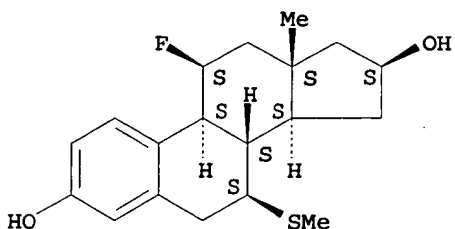
Absolute stereochemistry.



RN 287722-89-8 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-7-(methylthio)-,
(7 β ,11 β ,16 β)- (9CI) (CA INDEX NAME)

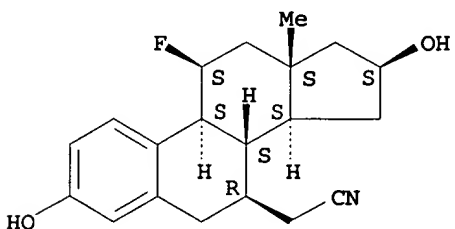
Absolute stereochemistry.



RN 287722-90-1 HCAPLUS

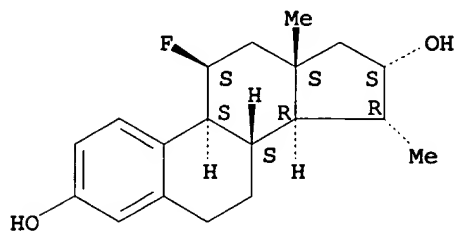
CN Estra-1,3,5(10)-triene-7-acetonitrile, 11-fluoro-3,16-dihydroxy-,
(7 β ,11 β ,16 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



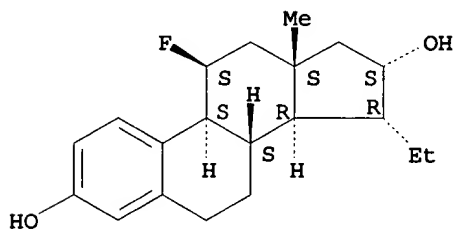
RN 287722-91-2 HCAPLUS
 CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-methyl-,
 (11 β ,15 α ,16 α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



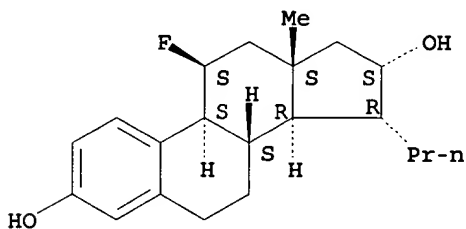
RN 287722-92-3 HCAPLUS
 CN Estra-1,3,5(10)-triene-3,16-diol, 15-ethyl-11-fluoro-,
 (11 β ,15 α ,16 α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



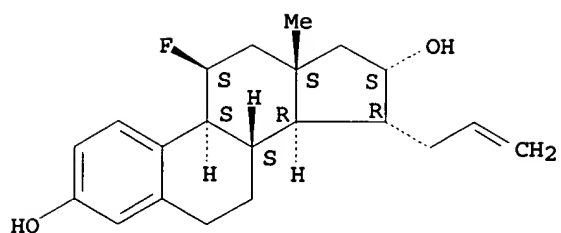
RN 287722-93-4 HCAPLUS
 CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-propyl-,
 (11 β ,15 α ,16 α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 287722-94-5 HCAPLUS
 CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-(2-propenyl)-,
 (11 β ,15 α ,16 α)- (9CI) (CA INDEX NAME)

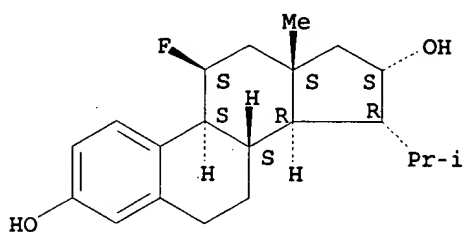
Absolute stereochemistry.



RN 287722-95-6 HCAPLUS

CN Estradiol, 11-fluoro-15-(1-methylethyl)-, (11 β ,15 α ,16 α)- (9CI) (CA INDEX NAME)

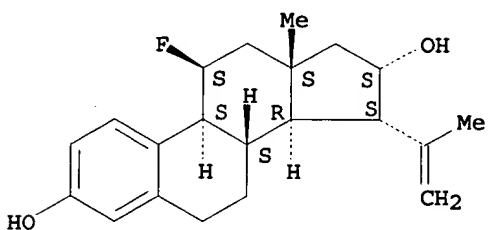
Absolute stereochemistry.



RN 287722-96-7 HCAPLUS

CN Estradiol, 11-fluoro-15-(1-methylethenyl)-, (11 β ,15 α ,16 α)- (9CI) (CA INDEX NAME)

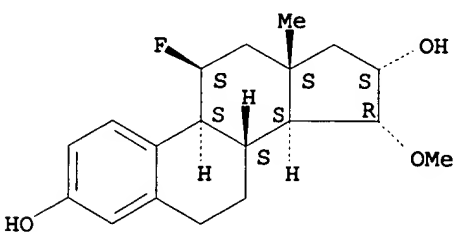
Absolute stereochemistry.



RN 287722-97-8 HCAPLUS

CN Estradiol, 11-fluoro-15-methoxy-, (11 β ,15 α ,16 α)- (9CI) (CA INDEX NAME)

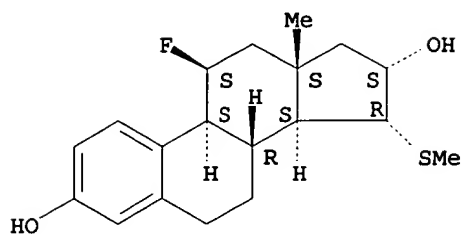
Absolute stereochemistry.



RN 287722-98-9 HCAPLUS

CN Estradiol, 11-fluoro-15-(methylthio)-, (11 β ,15 α ,16 α)- (9CI) (CA INDEX NAME)

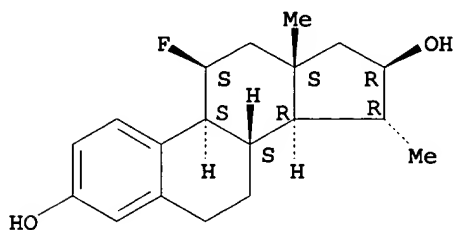
Absolute stereochemistry.



RN 287722-99-0 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-methyl-,
(11β,15α,16β)- (9CI) (CA INDEX NAME)

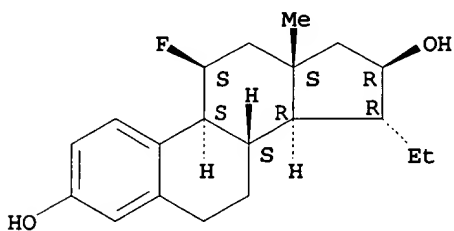
Absolute stereochemistry.



RN 287723-00-6 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 15-ethyl-11-fluoro-,
(11β,15α,16β)- (9CI) (CA INDEX NAME)

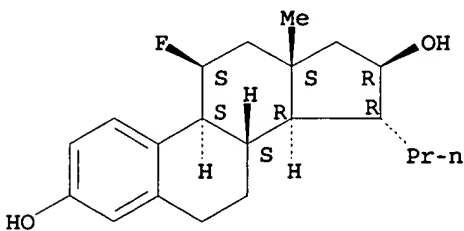
Absolute stereochemistry.



RN 287723-01-7 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-propyl-,
(11β,15α,16β)- (9CI) (CA INDEX NAME)

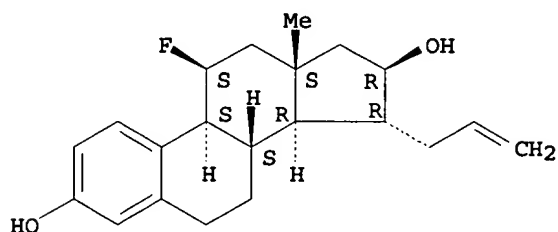
Absolute stereochemistry.



RN 287723-02-8 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-(2-propenyl)-,
(11 β ,15 α ,16 β)- (9CI) (CA INDEX NAME)

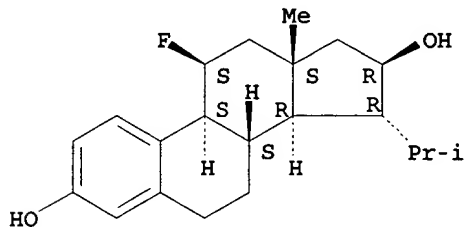
Absolute stereochemistry.



RN 287723-03-9 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-(1-methylethyl)-,
(11 β ,15 α ,16 β)- (9CI) (CA INDEX NAME)

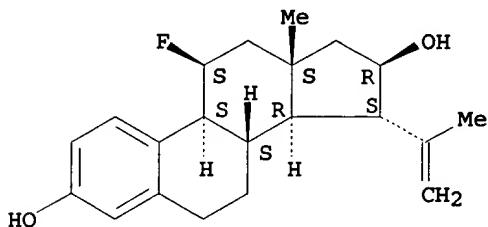
Absolute stereochemistry.



RN 287723-04-0 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-(1-methylethenyl)-,
(11 β ,15 α ,16 β)- (9CI) (CA INDEX NAME)

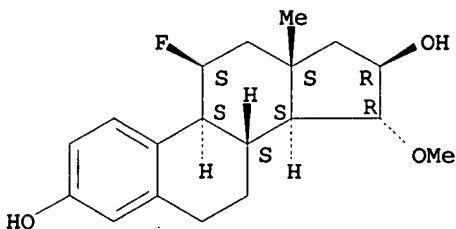
Absolute stereochemistry.



RN 287723-05-1 HCAPLUS

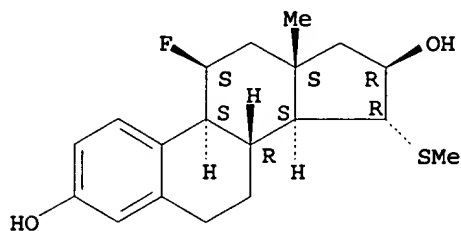
CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-methoxy-,
(11 β ,15 α ,16 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



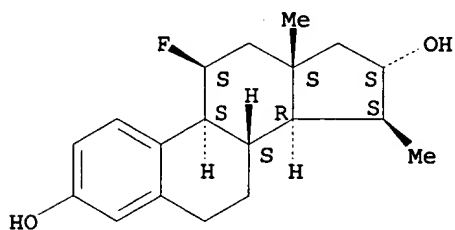
RN 287723-06-2 HCAPLUS
 CN Estr-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-(methylthio)-,
 (11 β ,15 α ,16 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



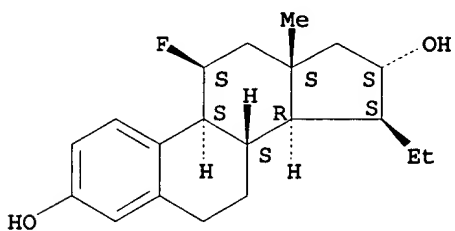
RN 287723-07-3 HCAPLUS
 CN Estr-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-methyl-,
 (11 β ,15 β ,16 α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



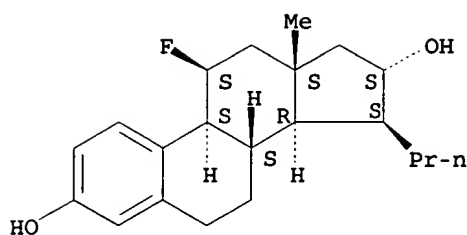
RN 287723-08-4 HCAPLUS
 CN Estr-1,3,5(10)-triene-3,16-diol, 15-ethyl-11-fluoro-,
 (11 β ,15 β ,16 α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 287723-09-5 HCAPLUS
 CN Estr-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-propyl-,
 (11 β ,15 β ,16 α)- (9CI) (CA INDEX NAME)

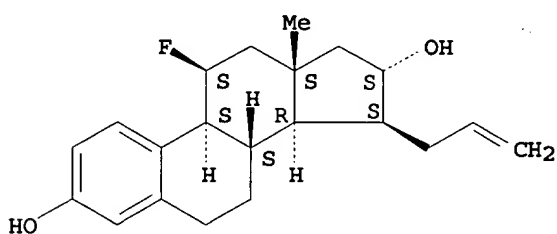
Absolute stereochemistry.



RN 287723-10-8 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-(2-propenyl)-,
(11β,15β,16α)- (9CI) (CA INDEX NAME)

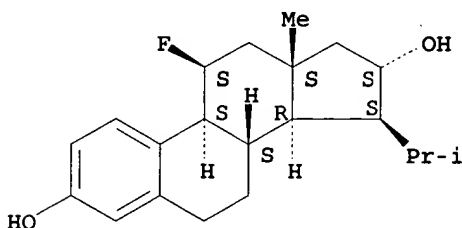
Absolute stereochemistry.



RN 287723-11-9 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-(1-methylethyl)-,
(11β,15β,16α)- (9CI) (CA INDEX NAME)

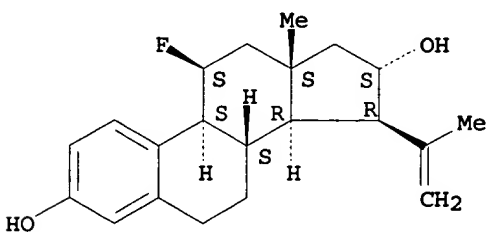
Absolute stereochemistry.



RN 287723-12-0 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-(1-methylethenyl)-,
(11β,15β,16α)- (9CI) (CA INDEX NAME)

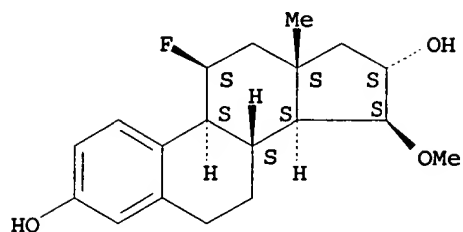
Absolute stereochemistry.



RN 287723-13-1 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-methoxy-,
(11β,15β,16α)- (9CI) (CA INDEX NAME)

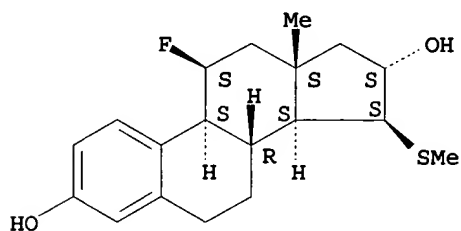
Absolute stereochemistry.



RN 287723-14-2 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-(methylthio)-,
(11β,15β,16α)- (9CI) (CA INDEX NAME)

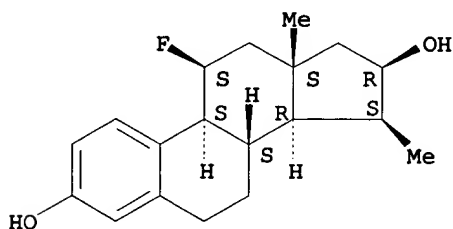
Absolute stereochemistry.



RN 287723-15-3 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-methyl-,
(11β,15β,16β)- (9CI) (CA INDEX NAME)

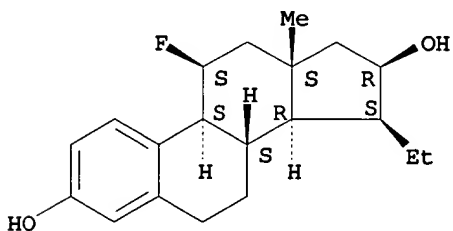
Absolute stereochemistry.



RN 287723-16-4 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 15-ethyl-11-fluoro-,
(11β,15β,16β)- (9CI) (CA INDEX NAME)

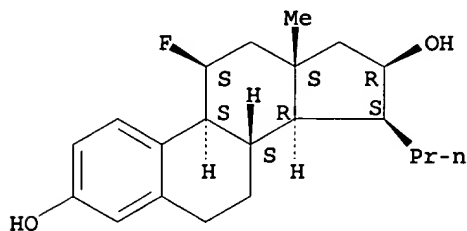
Absolute stereochemistry.



RN 287723-17-5 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-propyl-,
(11 β ,15 β ,16 β)- (9CI) (CA INDEX NAME)

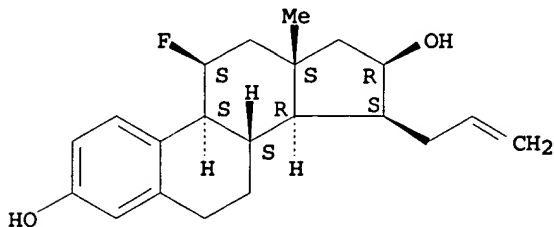
Absolute stereochemistry.



RN 287723-18-6 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-(2-propenyl)-,
(11 β ,15 β ,16 β)- (9CI) (CA INDEX NAME)

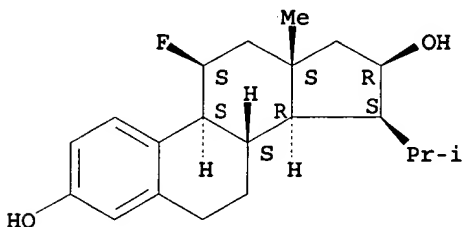
Absolute stereochemistry.



RN 287723-19-7 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-(1-methylethyl)-,
(11 β ,15 β ,16 β)- (9CI) (CA INDEX NAME)

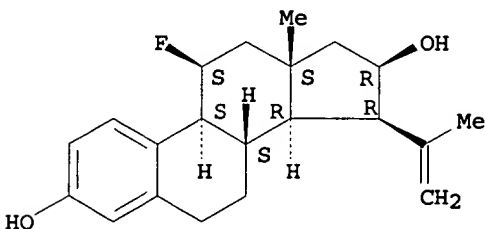
Absolute stereochemistry.



RN 287723-20-0 HCAPLUS

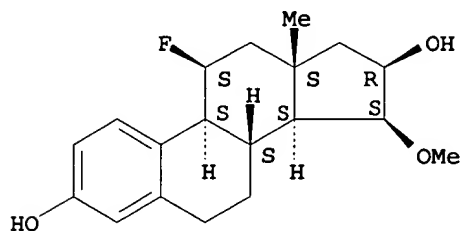
CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-(1-methylethenyl)-,
(11 β ,15 β ,16 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



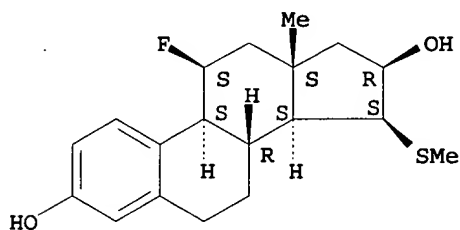
RN 287723-21-1 HCAPLUS
 CN Estr-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-methoxy-,
 (11 β ,15 β ,16 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



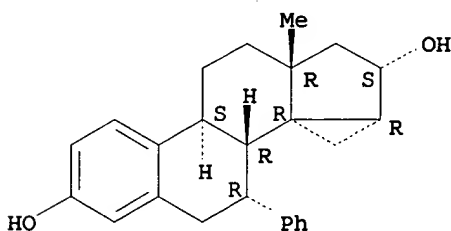
RN 287723-22-2 HCAPLUS
 CN Estr-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-(methylthio)-,
 (11 β ,15 β ,16 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



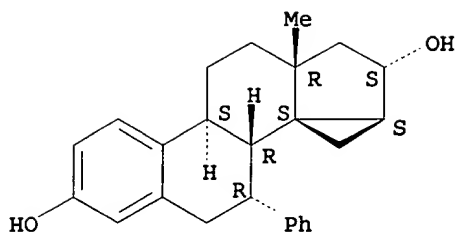
RN 287723-23-3 HCAPLUS
 CN Cycloprop[14,15]estra-1,3,5(10)-triene-3,16-diol,
 3',15-dihydro-7-phenyl-, (7 α ,14R,15 β ,16 α)- (9CI)
 (CA INDEX NAME)

Absolute stereochemistry.



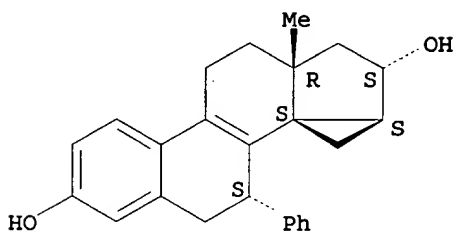
RN 287723-24-4 HCAPLUS
 CN Cycloprop[14,15]estra-1,3,5(10)-triene-3,16-diol,
 3',15-dihydro-7-phenyl-, (7 α ,14S,15 α ,16 α)- (9CI)
 (CA INDEX NAME)

Absolute stereochemistry.



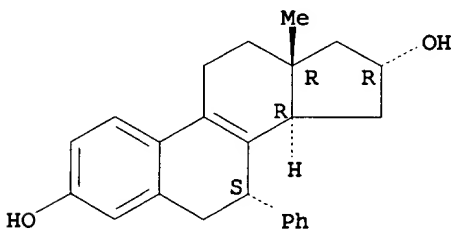
RN 287723-25-5 HCAPLUS
 CN Cycloprop[14,15]estra-1,3,5(10),8-tetraene-3,16-diol,
 3',15-dihydro-7-phenyl-, (7 α ,14S,15 α ,16 α)- (9CI)
 (CA INDEX NAME)

Absolute stereochemistry.



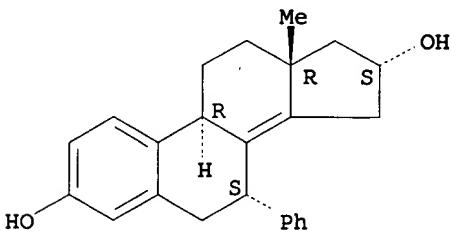
RN 287723-26-6 HCAPLUS
 CN Estra-1,3,5(10),8-tetraene-3,16-diol, 7-phenyl-,
 (7 α ,16 α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



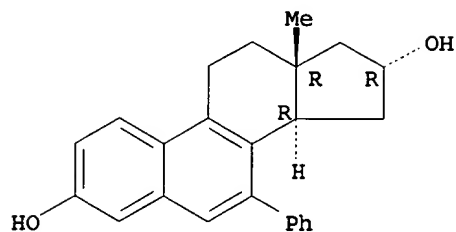
RN 287723-27-7 HCAPLUS
 CN Estra-1,3,5(10),8(14)-tetraene-3,16-diol, 7-phenyl-,
 (7 α ,16 α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



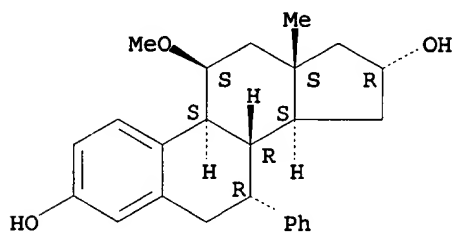
RN 287723-28-8 HCAPLUS
 CN Estra-1,3,5,7,9-pentaene-3,16-diol, 7-phenyl-, (16 α)- (9CI)

Absolute stereochemistry.



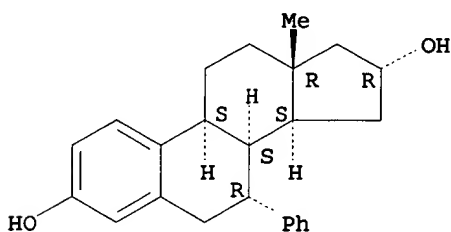
CN Estr-1,3,5(10)-triene-3,16-diol, 11-methoxy-7-phenyl-,
(7 α ,11 β ,16 α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



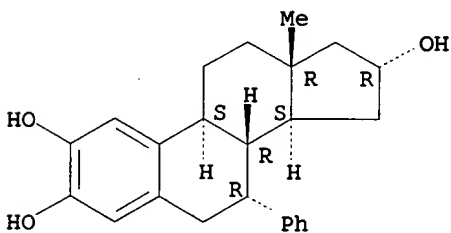
CN Estra-1,3,5(10)-triene-3,16-diol, 7-phenyl-,
 (7 α ,8 α ,16 α) - (9CI) (CA INDEX NAME)

Absolute stereochemistry.



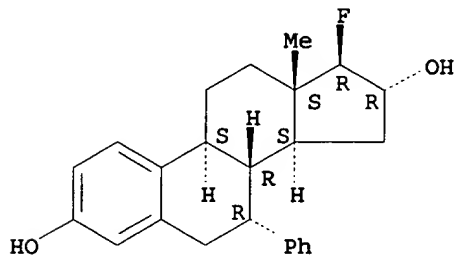
CN Estra-1,3,5(10)-triene-2,3,16-triol, 7-phenyl-,
 (7 α ,16 α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



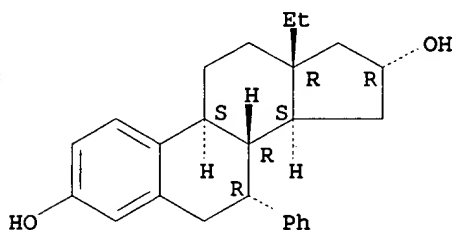
RN 287723-32-4 HCAPLUS
 CN Estra-1,3,5(10)-triene-3,16-diol, 17-fluoro-7-phenyl-,
 (7 α ,16 α ,17 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



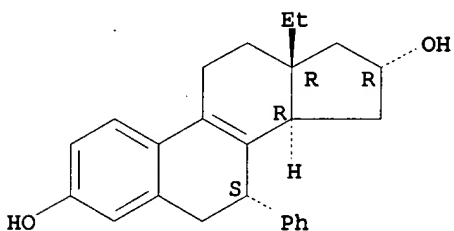
RN 287723-33-5 HCAPLUS
 CN Gona-1,3,5(10)-triene-3,16-diol, 13-ethyl-7-phenyl-,
 (7 α ,16 α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



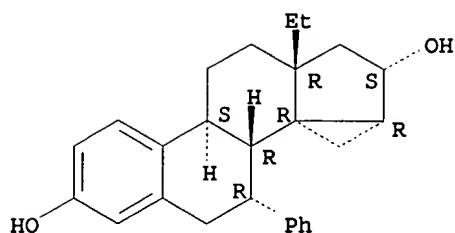
RN 287723-35-7 HCAPLUS
 CN Gona-1,3,5(10),8-tetraene-3,16-diol, 13-ethyl-7-phenyl-,
 (7 α ,16 α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 287723-37-9 HCAPLUS
 CN Cyclopropa[14,15]gona-1,3,5(10)-triene-3,16-diol,
 13-ethyl-3',15-dihydro-7-phenyl-, (7 α ,14R,15 β ,16 α) - (9CI) (CA INDEX NAME)

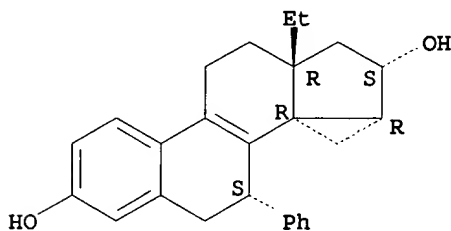
Absolute stereochemistry.



RN 287723-40-4 HCAPLUS

CN Cyclopropa[14,15]gona-1,3,5(10),8-tetraene-3,16-diol,
13-ethyl-3',15-dihydro-7-phenyl-, (7 α ,14R,15 β ,16 α) - (9CI) (CA INDEX NAME)

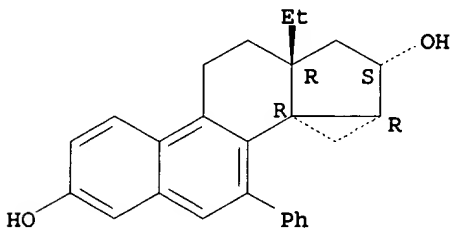
Absolute stereochemistry.



RN 287723-41-5 HCAPLUS

CN Cyclopropa[14,15]gona-1,3,5,7,9-pentaene-3,16-diol,
13-ethyl-3',15-dihydro-7-phenyl-, (14R,15 β ,16 α) - (9CI)
(CA INDEX NAME)

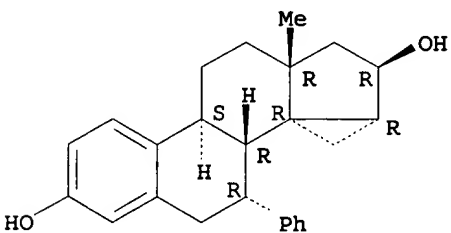
Absolute stereochemistry.



RN 287723-42-6 HCAPLUS

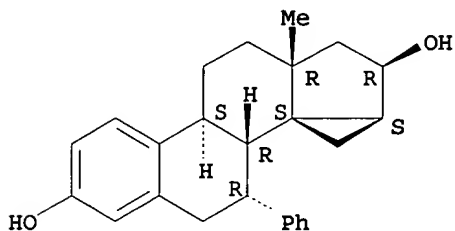
CN Cycloprop[14,15]estra-1,3,5(10)-triene-3,16-diol,
3',15-dihydro-7-phenyl-, (7 α ,14R,15 β ,16 β) - (9CI)
(CA INDEX NAME)

Absolute stereochemistry.



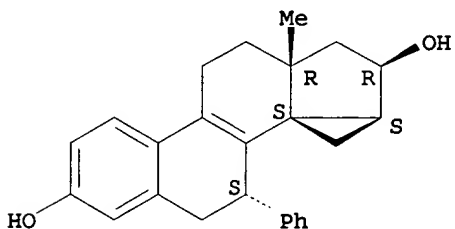
RN 287723-43-7 HCAPLUS
 CN Cycloprop[14,15]estra-1,3,5(10)-triene-3,16-diol,
 3',15-dihydro-7-phenyl-, (7 α ,14S,15 α ,16 β)- (9CI)
 (CA INDEX NAME)

Absolute stereochemistry.



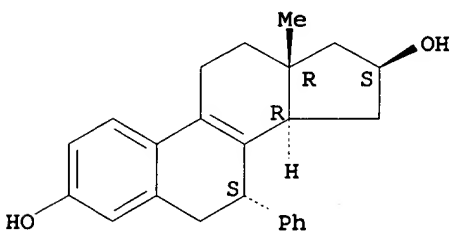
RN 287723-44-8 HCAPLUS
 CN Cycloprop[14,15]estra-1,3,5(10),8-tetraene-3,16-diol,
 3',15-dihydro-7-phenyl-, (7 α ,14S,15 α ,16 β)- (9CI)
 (CA INDEX NAME)

Absolute stereochemistry.



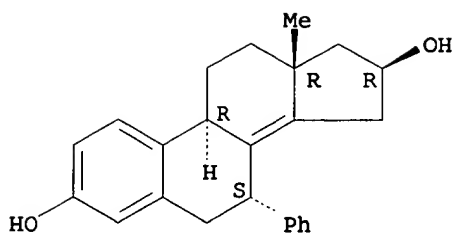
RN 287723-45-9 HCAPLUS
 CN Estra-1,3,5(10),8-tetraene-3,16-diol, 7-phenyl-,
 (7 α ,16 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



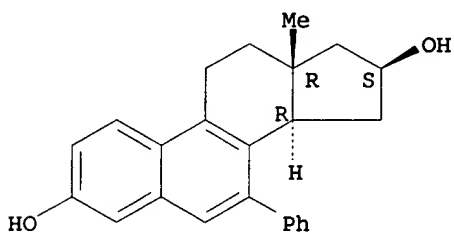
RN 287723-46-0 HCAPLUS
 CN Estra-1,3,5(10),8(14)-tetraene-3,16-diol, 7-phenyl-,
 (7 α ,16 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



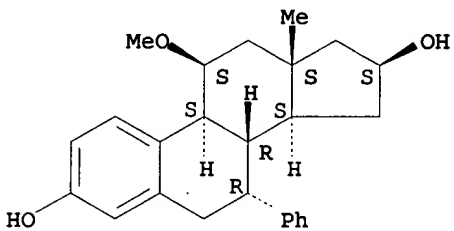
RN 287723-47-1 HCAPLUS
 CN Estra-1,3,5,7,9-pentaene-3,16-diol, 7-phenyl-, (16 β)- (9CI)
 (CA INDEX NAME)

Absolute stereochemistry.



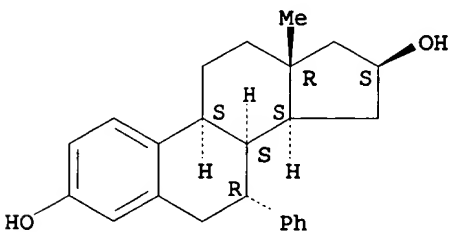
RN 287723-48-2 HCAPLUS
 CN Estra-1,3,5(10)-triene-3,16-diol, 11-methoxy-7-phenyl-,
 (7 α ,11 β ,16 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



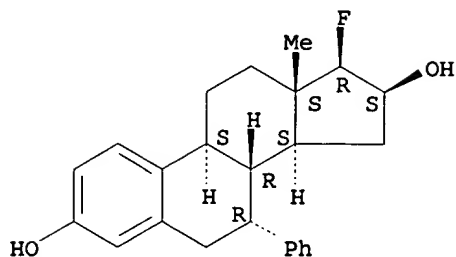
RN 287723-49-3 HCAPLUS
 CN Estra-1,3,5(10)-triene-3,16-diol, 7-phenyl-,
 (7 α ,8 α ,16 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



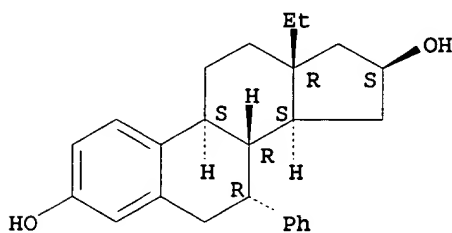
RN 287723-50-6 HCAPLUS
 CN Estra-1,3,5(10)-triene-3,16-diol, 17-fluoro-7-phenyl-,
 (7 α ,16 β ,17 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



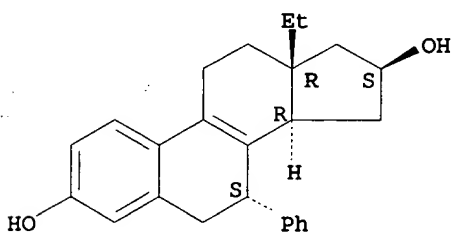
RN 287723-51-7 HCAPLUS
 CN Gona-1,3,5(10)-triene-3,16-diol, 13-ethyl-7-phenyl-,
 (7 α ,16 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



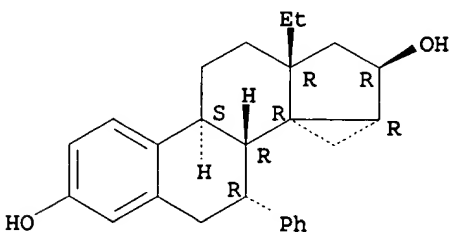
RN 287723-52-8 HCAPLUS
 CN Gona-1,3,5(10),8-tetraene-3,16-diol, 13-ethyl-7-phenyl-,
 (7 α ,16 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



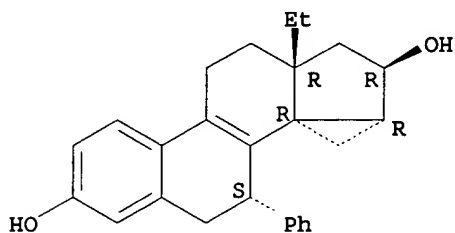
RN 287723-53-9 HCAPLUS
 CN Cyclopropa[14,15]gona-1,3,5(10)-triene-3,16-diol,
 13-ethyl-3',15-dihydro-7-phenyl-, (7 α ,14R,15 β ,16 β)-
 (9CI) (CA INDEX NAME)

Absolute stereochemistry.



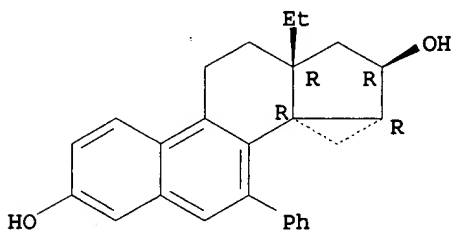
RN 287723-54-0 HCAPLUS
 CN Cyclopropa[14,15]gona-1,3,5(10),8-tetraene-3,16-diol,
 13-ethyl-3',15-dihydro-7-phenyl-, (7 α ,14R,15 β ,16 β)-
 (9CI) (CA INDEX NAME)

Absolute stereochemistry.



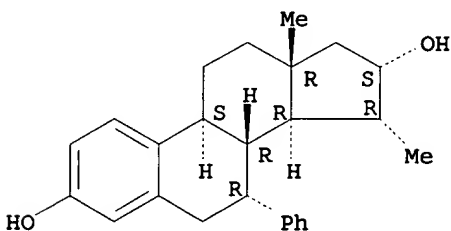
RN 287723-55-1 HCAPLUS
 CN Cyclopropa[14,15]gona-1,3,5,7,9-pentaene-3,16-diol,
 13-ethyl-3',15-dihydro-7-phenyl-, (14R,15 β ,16 β)- (9CI)
 (CA INDEX NAME)

Absolute stereochemistry.



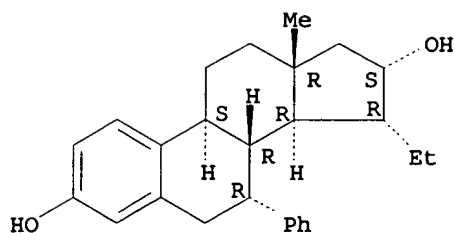
RN 287723-56-2 HCAPLUS
 CN Estra-1,3,5(10)-triene-3,16-diol, 15-methyl-7-phenyl-,
 (7 α ,15 α ,16 α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 287723-57-3 HCAPLUS
 CN Estra-1,3,5(10)-triene-3,16-diol, 15-ethyl-7-phenyl-,
 (7 α ,15 α ,16 α)- (9CI) (CA INDEX NAME)

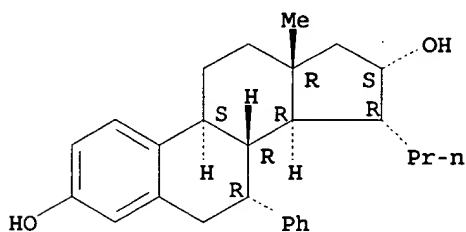
Absolute stereochemistry.



RN 287723-58-4 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 7-phenyl-15-propyl-,
(7 α ,15 α ,16 α)- (9CI) (CA INDEX NAME)

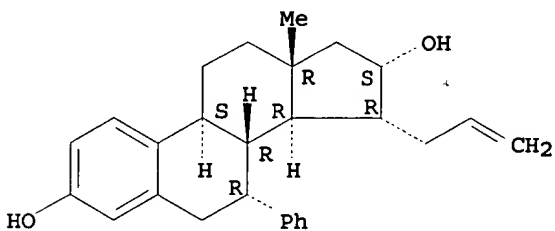
Absolute stereochemistry.



RN 287723-59-5 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 7-phenyl-15-(2-propenyl)-,
(7 α ,15 α ,16 α)- (9CI) (CA INDEX NAME)

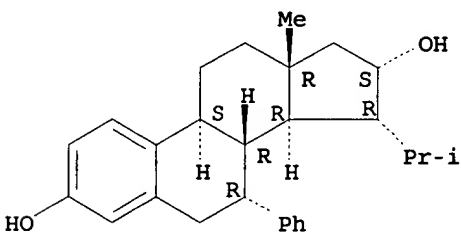
Absolute stereochemistry.



RN 287723-60-8 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 15-(1-methylethyl)-7-phenyl-,
(7 α ,15 α ,16 α)- (9CI) (CA INDEX NAME)

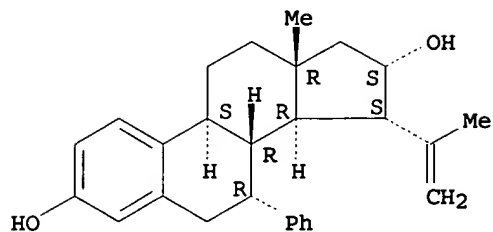
Absolute stereochemistry.



RN 287723-61-9 HCAPLUS

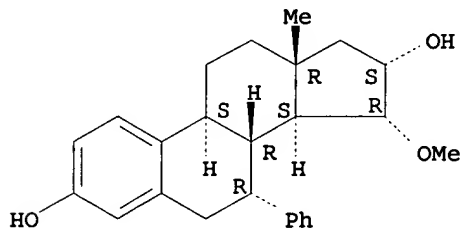
CN Estra-1,3,5(10)-triene-3,16-diol, 15-(1-methylethenyl)-7-phenyl-,
(7 α ,15 α ,16 α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



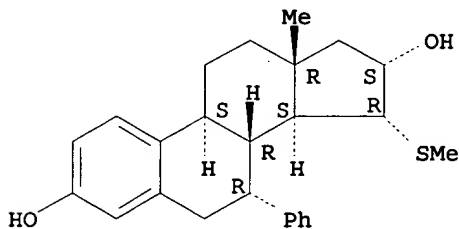
RN 287723-62-0 HCAPLUS
 CN Estradiol, 15-methoxy-7-phenyl-,
 (7 α ,15 α ,16 α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



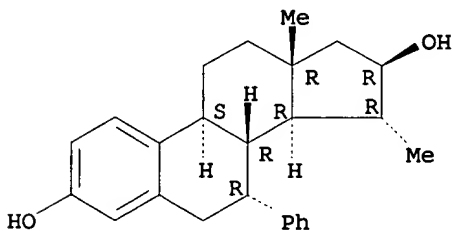
RN 287723-63-1 HCAPLUS
 CN Estradiol, 15-(methylthio)-7-phenyl-,
 (7 α ,15 α ,16 α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 287723-64-2 HCAPLUS
 CN Estradiol, 15-methyl-7-phenyl-,
 (7 α ,15 α ,16 β)- (9CI) (CA INDEX NAME)

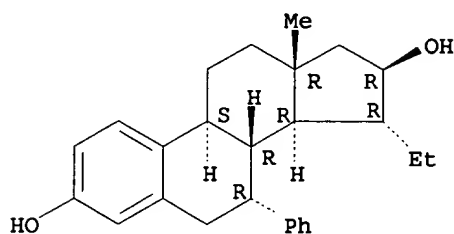
Absolute stereochemistry.



RN 287723-65-3 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 15-ethyl-7-phenyl-,
(7 α ,15 α ,16 β)- (9CI) (CA INDEX NAME)

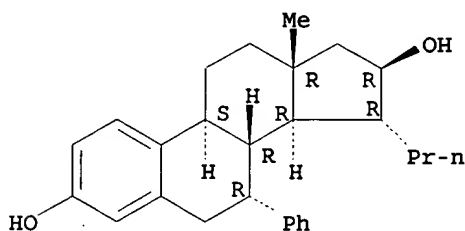
Absolute stereochemistry.



RN 287723-66-4 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 7-phenyl-15-propyl-,
(7 α ,15 α ,16 β)- (9CI) (CA INDEX NAME)

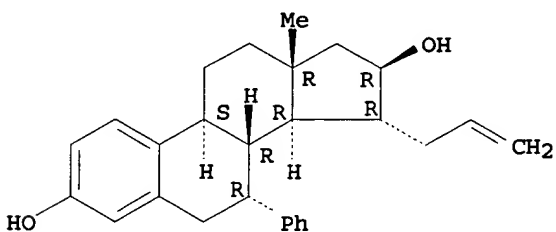
Absolute stereochemistry.



RN 287723-67-5 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 7-phenyl-15-(2-propenyl)-,
(7 α ,15 α ,16 β)- (9CI) (CA INDEX NAME)

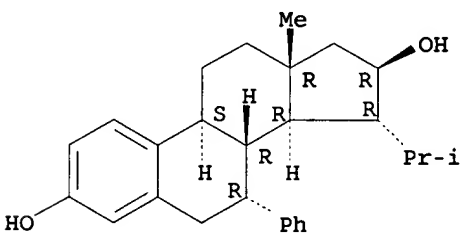
Absolute stereochemistry.



RN 287723-68-6 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 15-(1-methylethyl)-7-phenyl-,
(7 α ,15 α ,16 β)- (9CI) (CA INDEX NAME)

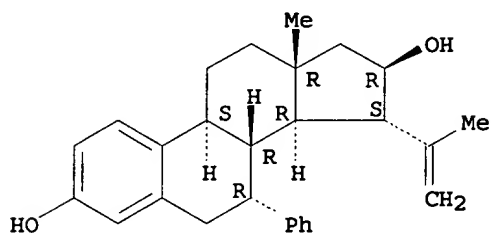
Absolute stereochemistry.



RN 287723-69-7 HCAPLUS

CN Estr-1,3,5(10)-triene-3,16-diol, 15-(1-methylethenyl)-7-phenyl-,
(7 α ,15 α ,16 β)- (9CI) (CA INDEX NAME)

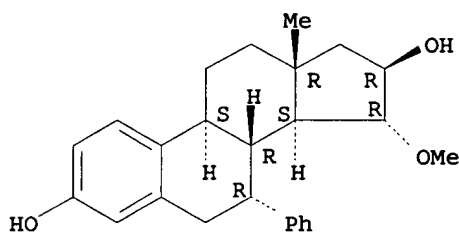
Absolute stereochemistry.



RN 287723-70-0 HCAPLUS

CN Estr-1,3,5(10)-triene-3,16-diol, 15-methoxy-7-phenyl-,
(7 α ,15 α ,16 β)- (9CI) (CA INDEX NAME)

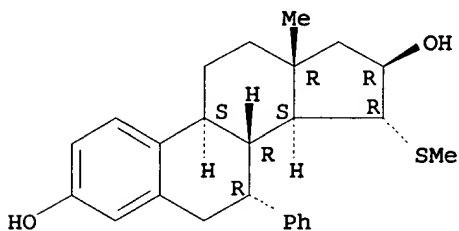
Absolute stereochemistry.



RN 287723-71-1 HCAPLUS

CN Estr-1,3,5(10)-triene-3,16-diol, 15-(methylthio)-7-phenyl-,
(7 α ,15 α ,16 β)- (9CI) (CA INDEX NAME)

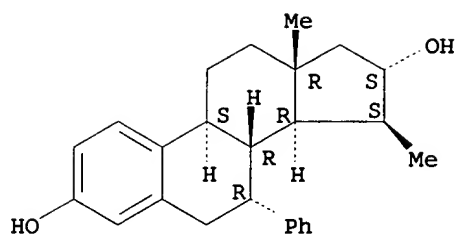
Absolute stereochemistry.



RN 287723-72-2 HCAPLUS

CN Estr-1,3,5(10)-triene-3,16-diol, 15-methyl-7-phenyl-,
(7 α ,15 β ,16 α)- (9CI) (CA INDEX NAME)

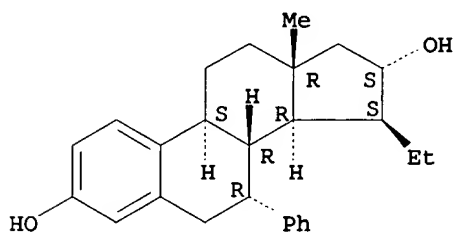
Absolute stereochemistry.



RN 287723-73-3 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 15-ethyl-7-phenyl-,
(7 α ,15 β ,16 α)- (9CI) (CA INDEX NAME)

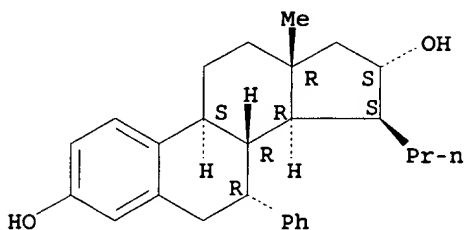
Absolute stereochemistry.



RN 287723-75-5 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 7-phenyl-15-propyl-,
(7 α ,15 β ,16 α)- (9CI) (CA INDEX NAME)

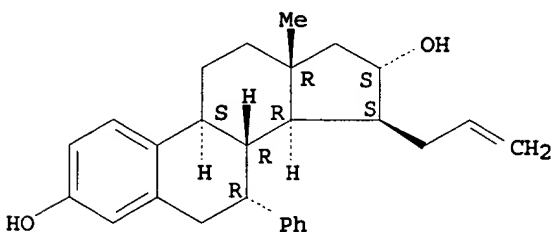
Absolute stereochemistry.



RN 287723-77-7 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 7-phenyl-15-(2-propenyl)-,
(7 α ,15 β ,16 α)- (9CI) (CA INDEX NAME)

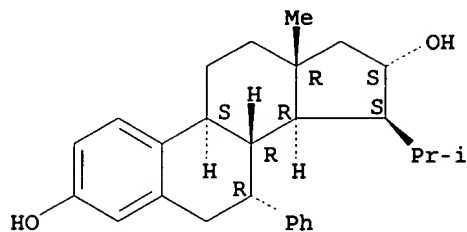
Absolute stereochemistry.



RN 287723-79-9 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 15-(1-methylethyl)-7-phenyl-,
(7 α ,15 β ,16 α)- (9CI) (CA INDEX NAME)

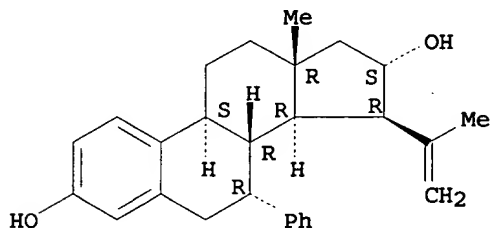
Absolute stereochemistry.



RN 287723-80-2 HCAPLUS

CN Estradiol, 15-(1-methylethenyl)-7-phenyl-,
(7 α ,15 β ,16 α)- (9CI) (CA INDEX NAME)

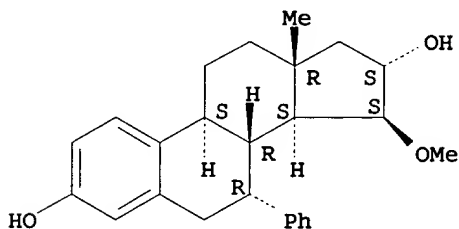
Absolute stereochemistry.



RN 287723-81-3 HCAPLUS

CN Estradiol, 15-methoxy-7-phenyl-,
(7 α ,15 β ,16 α)- (9CI) (CA INDEX NAME)

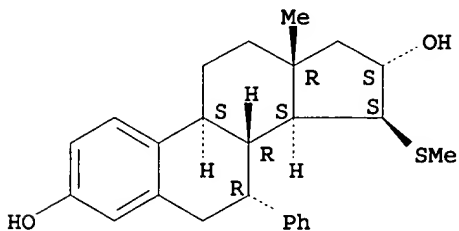
Absolute stereochemistry.



RN 287723-82-4 HCAPLUS

CN Estradiol, 15-(methylthio)-7-phenyl-,
(7 α ,15 β ,16 α)- (9CI) (CA INDEX NAME)

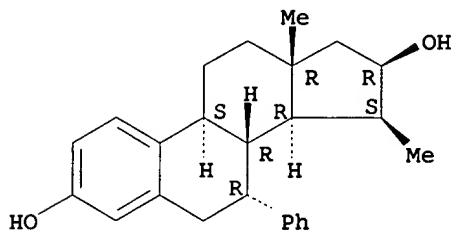
Absolute stereochemistry.



RN 287723-83-5 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 15-methyl-7-phenyl-,
(7 α ,15 β ,16 β)- (9CI) (CA INDEX NAME)

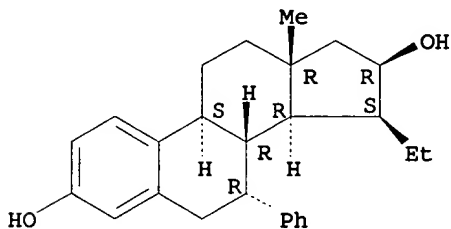
Absolute stereochemistry.



RN 287723-84-6 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 15-ethyl-7-phenyl-,
(7 α ,15 β ,16 β)- (9CI) (CA INDEX NAME)

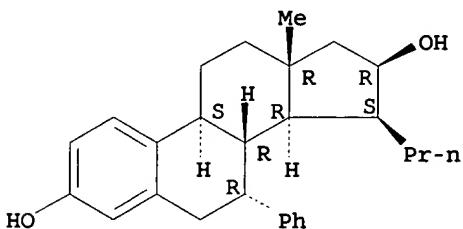
Absolute stereochemistry.



RN 287723-85-7 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 7-phenyl-15-propyl-,
(7 α ,15 β ,16 β)- (9CI) (CA INDEX NAME)

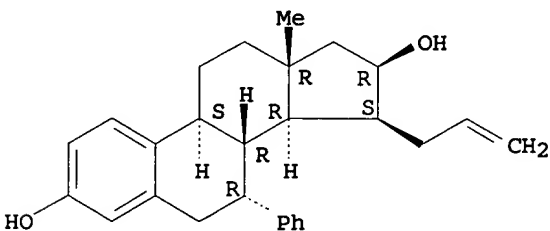
Absolute stereochemistry.



RN 287723-86-8 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 7-phenyl-15-(2-propenyl)-,
(7 α ,15 β ,16 β)- (9CI) (CA INDEX NAME)

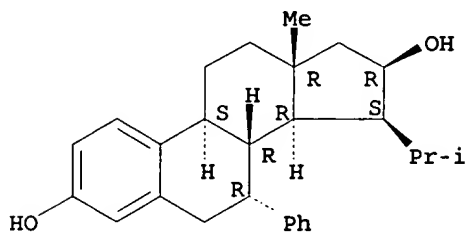
Absolute stereochemistry.



RN 287723-87-9 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 15-(1-methylethyl)-7-phenyl-,
(7 α ,15 β ,16 β)- (9CI) (CA INDEX NAME)

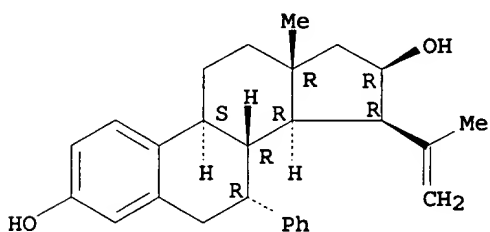
Absolute stereochemistry.



RN 287723-88-0 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 15-(1-methylethenyl)-7-phenyl-,
(7 α ,15 β ,16 β)- (9CI) (CA INDEX NAME)

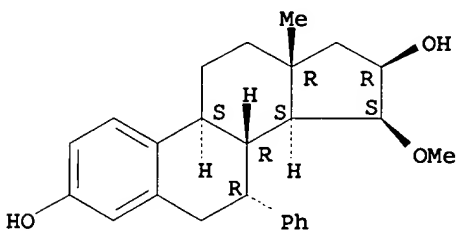
Absolute stereochemistry.



RN 287723-89-1 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 15-methoxy-7-phenyl-,
(7 α ,15 β ,16 β)- (9CI) (CA INDEX NAME)

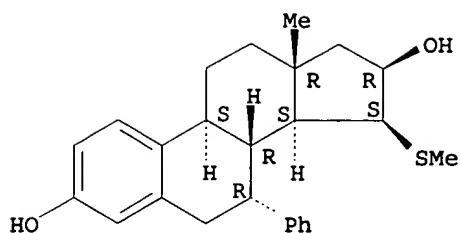
Absolute stereochemistry.



RN 287723-90-4 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 15-(methylthio)-7-phenyl-,
(7 α ,15 β ,16 β)- (9CI) (CA INDEX NAME)

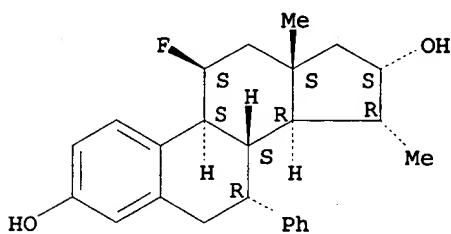
Absolute stereochemistry.



RN 287723-91-5 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-methyl-7-phenyl-,
(7 α ,11 β ,15 α ,16 α)- (9CI) (CA INDEX NAME)

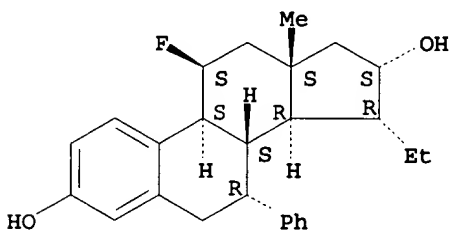
Absolute stereochemistry.



RN 287723-92-6 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 15-ethyl-11-fluoro-7-phenyl-,
(7 α ,11 β ,15 α ,16 α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 287723-93-7P 287723-94-8P 287723-95-9P
287723-96-0P 287723-97-1P 287723-98-2P
287723-99-3P 287724-00-9P 287724-01-0P
287724-02-1P 287724-03-2P 287724-04-3P
287724-05-4P 287724-06-5P 287724-07-6P
287724-08-7P 287724-09-8P 287724-10-1P
287724-11-2P 287724-12-3P 287724-13-4P
287724-14-5P 287724-15-6P 287724-16-7P
287724-17-8P 287724-18-9P 287724-19-0P
287724-20-3P 287724-21-4P 287724-22-5P
287724-23-6P 287724-24-7P

RL: BAC (Biological activity or effector, except adverse); BSU
(Biological study, unclassified); SPN (Synthetic preparation);

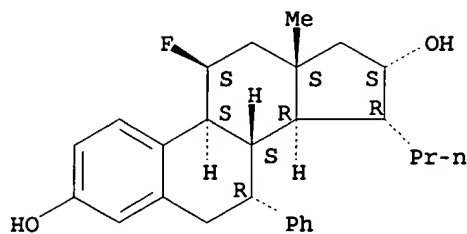
THU (Therapeutic use); BIOL (Biological study); PREP
(Preparation); USES (Uses)

(synthesis of 16-Hydroxyestratrienes as selectively effective
estrogens)

RN 287723-93-7 HCAPLUS

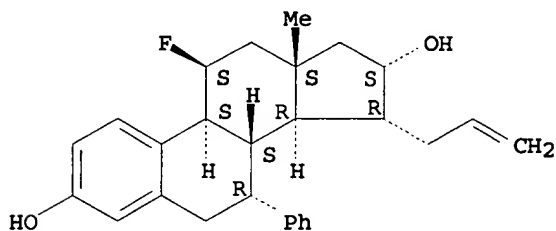
CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-7-phenyl-15-propyl-,
(7 α ,11 β ,15 α ,16 α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



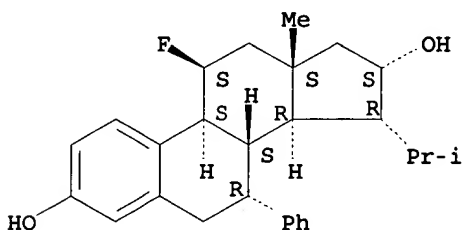
RN 287723-94-8 HCAPLUS
 CN Estradiol, 11-fluoro-7-phenyl-15-(2-propenyl)-, (7 α ,11 β ,15 α ,16 α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



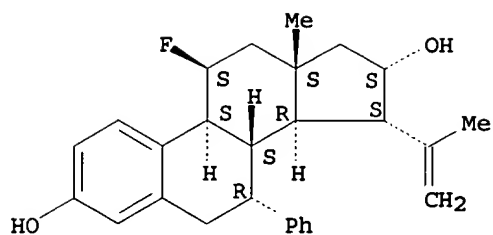
RN 287723-95-9 HCAPLUS
 CN Estradiol, 11-fluoro-15-(1-methylethyl)-7-phenyl-, (7 α ,11 β ,15 α ,16 α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 287723-96-0 HCAPLUS
 CN Estradiol, 11-fluoro-15-(1-methylethenyl)-7-phenyl-, (7 α ,11 β ,15 α ,16 α)- (9CI) (CA INDEX NAME)

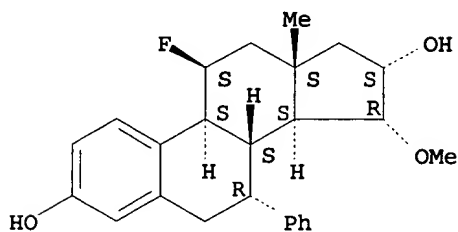
Absolute stereochemistry.



RN 287723-97-1 HCAPLUS

CN Estradiol, 11-fluoro-15-methoxy-7-phenyl-, (7 α ,11 β ,15 α ,16 α)- (9CI) (CA INDEX NAME)

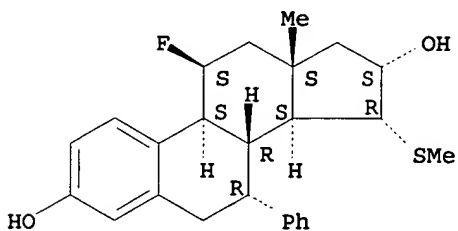
Absolute stereochemistry.



RN 287723-98-2 HCAPLUS

CN Estradiol, 11-fluoro-15-(methylthio)-7-phenyl-, (7 α ,11 β ,15 α ,16 α)- (9CI) (CA INDEX NAME)

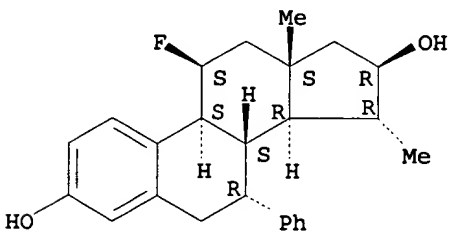
Absolute stereochemistry.



RN 287723-99-3 HCAPLUS

CN Estradiol, 11-fluoro-15-methyl-7-phenyl-, (7 α ,11 β ,15 α ,16 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

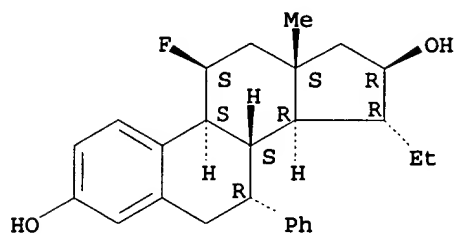


RN 287724-00-9 HCAPLUS

CN Estradiol, 15-ethyl-11-fluoro-7-phenyl-, (7 α ,11 β ,15 α ,16 β)- (9CI) (CA INDEX NAME)

(7 α ,11 β ,15 α ,16 β) - (9CI) (CA INDEX NAME)

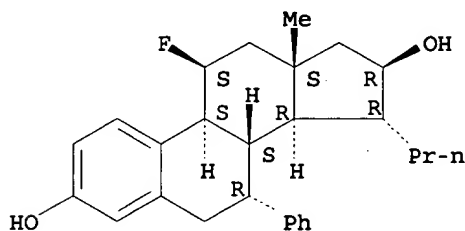
Absolute stereochemistry.



RN 287724-01-0 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-7-phenyl-15-propyl-,
(7 α ,11 β ,15 α ,16 β) - (9CI) (CA INDEX NAME)

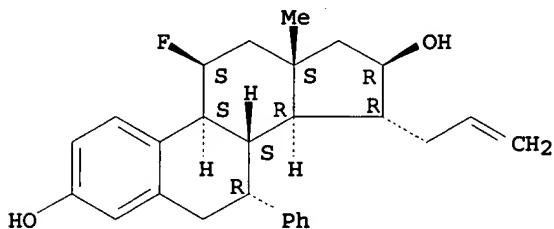
Absolute stereochemistry.



RN 287724-02-1 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-7-phenyl-15-(2-propenyl)-,
(7 α ,11 β ,15 α ,16 β) - (9CI) (CA INDEX NAME)

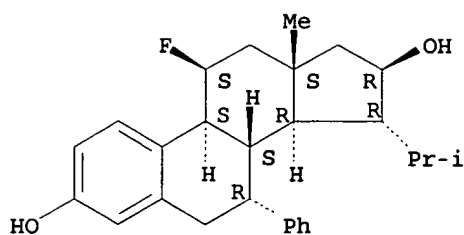
Absolute stereochemistry.



RN 287724-03-2 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-(1-methylethyl)-7-phenyl-,
(7 α ,11 β ,15 α ,16 β) - (9CI) (CA INDEX NAME)

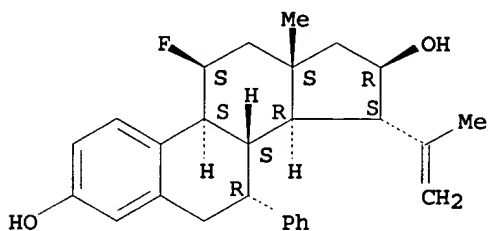
Absolute stereochemistry.



RN 287724-04-3 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-(1-methylethenyl)-7-phenyl-, (7 α ,11 β ,15 α ,16 β)- (9CI) (CA INDEX NAME)

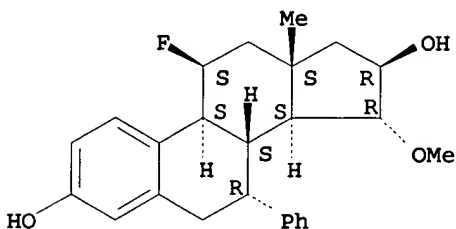
Absolute stereochemistry.



RN 287724-05-4 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-methoxy-7-phenyl-, (7 α ,11 β ,15 α ,16 β)- (9CI) (CA INDEX NAME)

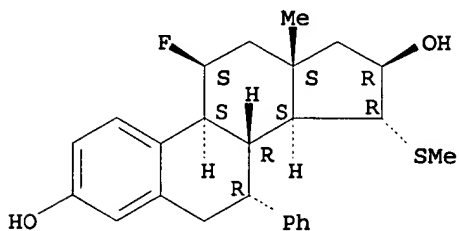
Absolute stereochemistry.



RN 287724-06-5 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-(methylthio)-7-phenyl-, (7 α ,11 β ,15 α ,16 β)- (9CI) (CA INDEX NAME)

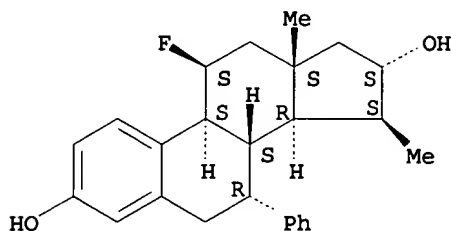
Absolute stereochemistry.



RN 287724-07-6 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-methyl-7-phenyl-,
(7 α ,11 β ,15 β ,16 α)- (9CI) (CA INDEX NAME)

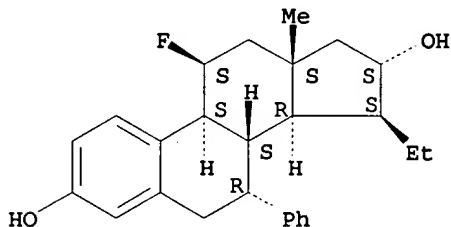
Absolute stereochemistry.



RN 287724-08-7 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 15-ethyl-11-fluoro-7-phenyl-,
(7 α ,11 β ,15 β ,16 α)- (9CI) (CA INDEX NAME)

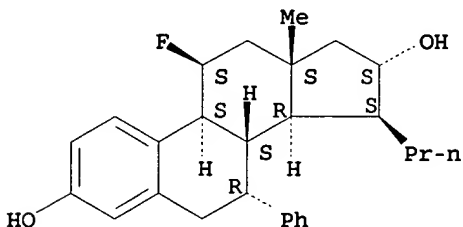
Absolute stereochemistry.



RN 287724-09-8 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-7-phenyl-15-propyl-,
(7 α ,11 β ,15 β ,16 α)- (9CI) (CA INDEX NAME)

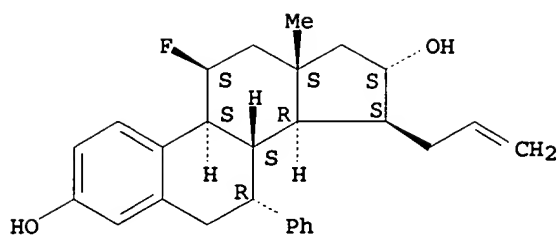
Absolute stereochemistry.



RN 287724-10-1 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-7-phenyl-15-(2-propenyl)-,
(7 α ,11 β ,15 β ,16 α)- (9CI) (CA INDEX NAME)

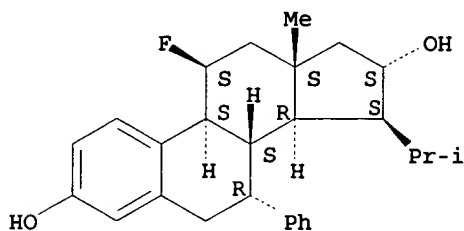
Absolute stereochemistry.



RN 287724-11-2 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-(1-methylethyl)-7-phenyl-, (7 α ,11 β ,15 β ,16 α)- (9CI) (CA INDEX NAME)

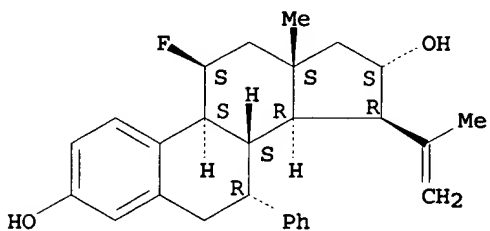
Absolute stereochemistry.



RN 287724-12-3 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-(1-methylethenyl)-7-phenyl-, (7 α ,11 β ,15 β ,16 α)- (9CI) (CA INDEX NAME)

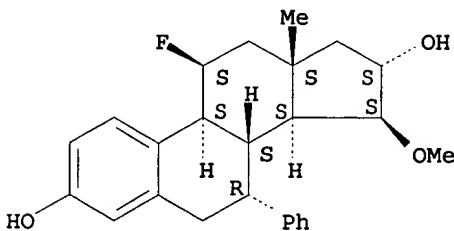
Absolute stereochemistry.



RN 287724-13-4 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-methoxy-7-phenyl-, (7 α ,11 β ,15 β ,16 α)- (9CI) (CA INDEX NAME)

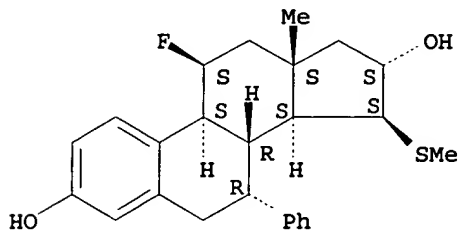
Absolute stereochemistry.



RN 287724-14-5 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-(methylthio)-7-phenyl-, (7 α ,11 β ,15 β ,16 α)- (9CI) (CA INDEX NAME)

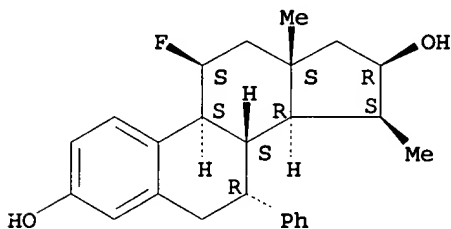
Absolute stereochemistry.



RN 287724-15-6 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-methyl-7-phenyl-, (7 α ,11 β ,15 β ,16 β)- (9CI) (CA INDEX NAME)

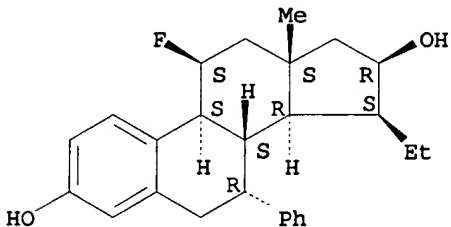
Absolute stereochemistry.



RN 287724-16-7 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 15-ethyl-11-fluoro-7-phenyl-, (7 α ,11 β ,15 β ,16 β)- (9CI) (CA INDEX NAME)

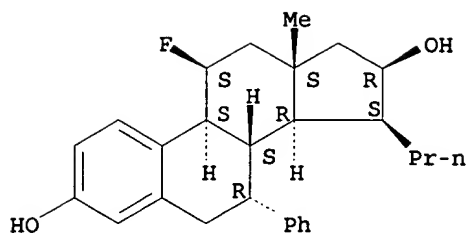
Absolute stereochemistry.



RN 287724-17-8 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-7-phenyl-15-propyl-, (7 α ,11 β ,15 β ,16 β)- (9CI) (CA INDEX NAME)

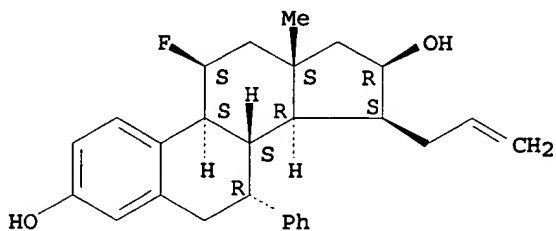
Absolute stereochemistry.



RN 287724-18-9 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-7-phenyl-15-(2-propenyl)-, (7 α ,11 β ,15 β ,16 β)- (9CI) (CA INDEX NAME)

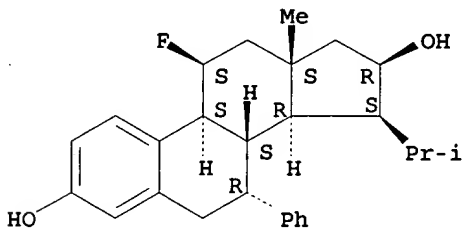
Absolute stereochemistry.



RN 287724-19-0 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-(1-methylethyl)-7-phenyl-, (7 α ,11 β ,15 β ,16 β)- (9CI) (CA INDEX NAME)

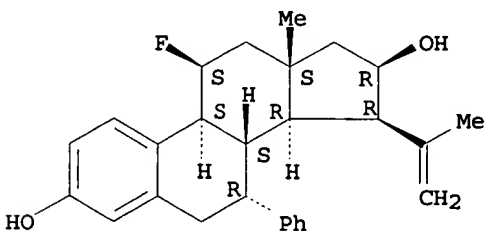
Absolute stereochemistry.



RN 287724-20-3 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-(1-methylethenyl)-7-phenyl-, (7 α ,11 β ,15 β ,16 β)- (9CI) (CA INDEX NAME)

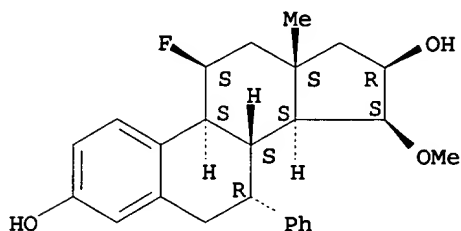
Absolute stereochemistry.



RN 287724-21-4 HCAPLUS

CN Estr-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-methoxy-7-phenyl-,
(7 α ,11 β ,15 β ,16 β)- (9CI) (CA INDEX NAME)

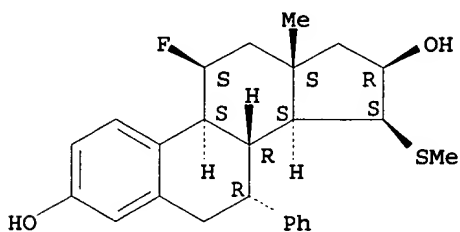
Absolute stereochemistry.



RN 287724-22-5 HCAPLUS

CN Estr-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-(methylthio)-7-phenyl-,
(7 α ,11 β ,15 β ,16 β)- (9CI) (CA INDEX NAME)

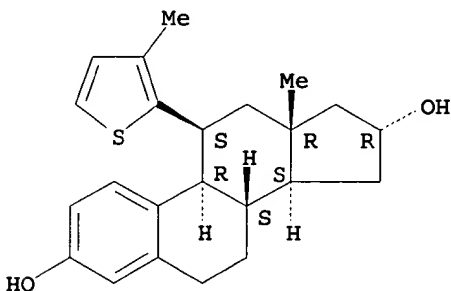
Absolute stereochemistry.



RN 287724-23-6 HCAPLUS

CN Estr-1,3,5(10)-triene-3,16-diol, 11-(3-methyl-2-thienyl)-,
(11 β ,16 α)- (9CI) (CA INDEX NAME)

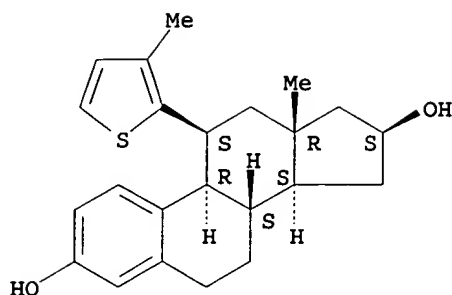
Absolute stereochemistry.



RN 287724-24-7 HCAPLUS

CN Estr-1,3,5(10)-triene-3,16-diol, 11-(3-methyl-2-thienyl)-,
(11 β ,16 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 1225-58-7

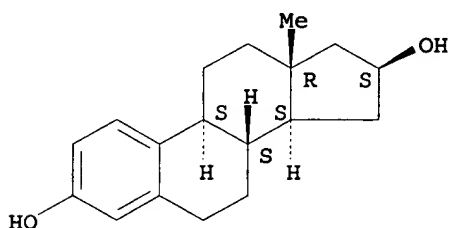
RL: RCT (Reactant); RACT (Reactant or reagent)

(synthesis of 16-Hydroxyestratrienes as selectively effective **estrogens**)

RN 1225-58-7 HCAPLUS

CN Estratriene-1,3,5(10)-triene-3,16-diol, (16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IC ICM C07J009-00

ICS C07J001-00; A61K031-565; A61K031-575

CC 32-3 (Steroids)

Section cross-reference(s): 1, 63

ST estratriene hydroxy analog prepn **estrogen** therapy

IT Prostate gland

(benign hyperplasia; synthesis of 16-Hydroxyestratrienes as selectively effective **estrogens**)

IT Uterus, neoplasm

(cervix, carcinoma, intraepithelial; synthesis of 16-Hydroxyestratrienes as selectively effective **estrogens**)

IT **Estrogens**

(deficiency; synthesis of 16-Hydroxyestratrienes as selectively effective **estrogens**)

IT Nervous system

(degeneration; synthesis of 16-Hydroxyestratrienes as selectively effective **estrogens**)

IT Immunity

(disorder; synthesis of 16-Hydroxyestratrienes as selectively effective **estrogens**)

IT Fertility

(female, disorder; synthesis of 16-Hydroxyestratrienes as selectively effective **estrogens**)

IT Artery, disease

(intima, hyperplasia; synthesis of 16-Hydroxyestratrienes as selectively effective **estrogens**)

IT Fertility

(male, disorder; synthesis of 16-Hydroxyestratrienes as selectively effective **estrogens**)

IT Menopause

(perimenopause; synthesis of 16-Hydroxyestratrienes as selectively effective **estrogens**)

IT Menopause
(postmenopause; synthesis of 16-Hydroxyestratrienes as selectively effective **estrogens**)

IT Alzheimer's disease
Arteriosclerosis
Blood vessel, disease
Heart, disease
Hormone replacement therapy
Ovary, disease
(synthesis of 16-Hydroxyestratrienes as selectively effective **estrogens**)

IT Osteoporosis
(therapeutic agents; synthesis of 16-Hydroxyestratrienes as selectively effective **estrogens**)

IT 109932-04-9P 110012-46-9P 287721-55-5P
287721-56-6P 287721-57-7P 287721-58-8P
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287721-65-7P 287721-66-8P 287721-67-9P
287721-68-0P 287721-69-1P 287721-70-4P
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287721-74-8P 287721-75-9P 287721-76-0P
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 287723-87-9P 287723-88-0P 287723-89-1P
 287723-90-4P 287723-91-5P 287723-92-6P

RL: BAC (Biological activity or effector, except adverse); BSU
 (Biological study, unclassified); SPN (Synthetic preparation);
 THU (Therapeutic use); BIOL (Biological study); PREP
 (Preparation); USES (Uses)

(synthesis of 16-Hydroxyestratrienes as selectively effective
 estrogens)

IT 287723-93-7P 287723-94-8P 287723-95-9P
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 287724-20-3P 287724-21-4P 287724-22-5P
 287724-23-6P 287724-24-7P

RL: BAC (Biological activity or effector, except adverse); BSU
 (Biological study, unclassified); SPN (Synthetic preparation);
 THU (Therapeutic use); BIOL (Biological study); PREP
 (Preparation); USES (Uses)

(synthesis of 16-Hydroxyestratrienes as selectively effective
 estrogens)

IT 1225-58-7 10449-00-0 13639-96-8 13865-88-8
 59126-71-5

RL: RCT (Reactant); RACT (Reactant or reagent)

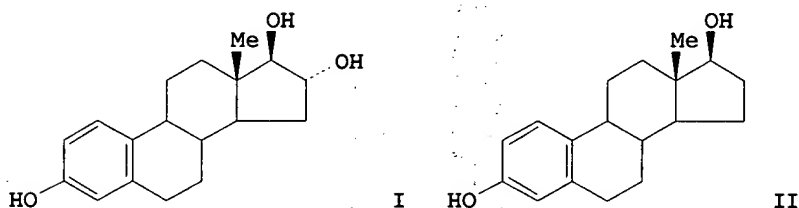
(synthesis of 16-Hydroxyestratrienes as selectively effective
 estrogens)

IT 287724-25-8P 287724-26-9P 287724-27-0P 287724-28-1P
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 287724-41-8P 287724-42-9P 287726-67-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP
 (Preparation); RACT (Reactant or reagent)

(synthesis of 16-Hydroxyestratrienes as selectively effective
 estrogens)

L52 ANSWER 2 OF 24 HCAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 1990:801 HCAPLUS
 DOCUMENT NUMBER: 112:801
 TITLE: Relative mitogenic activities of various
 estrogens and antiestrogens
 AUTHOR(S): Stack, Gary; Korach, Kenneth; Gorski, Jack
 CORPORATE SOURCE: Coll. Agric. Life Sci., Univ. Wisconsin,
 Madison, WI, 53706, USA
 SOURCE: Steroids (1989), 54(2), 227-43
 CODEN: STEDAM; ISSN: 0039-128X
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



AB The abilities of a variety of estrogens and antiestrogens to stimulate DNA synthesis in the prepuberal rat uterus were compared. One microgram of each compound was administered in vivo via a single i.p. injection. DNA synthesis was assayed in vitro in isolated nuclei 24 h later. The relative mitogenicities of the steroidal estrogens were : 16 α -estradiol < 17 α -estradiol = estriol (I) = 16-epiestriol < 16 β -estradiol = 17 β -estradiol (II). The potencies of several nonsteroidal estrogens were also tested. Indenestrol A was as potent as II, whereas indanestrol and dimethylstilbestrol had weaker activities. The antiestrogens, nafoxidine and 4-hydroxytamoxifen, were both potent stimulators of DNA synthesis. The abilities of an estrogen to stimulate increases in uterine wet weight, DNA polymerase α activities, and DNA synthesis in uterine nuclei 24 h after injection were closely correlated. Because the magnitude of the stimulation of DNA synthesis was greatest, its measurement is the most sensitive of these assays, of uterotrophic activity.

IT 1225-58-7, 16 β -Estradiol

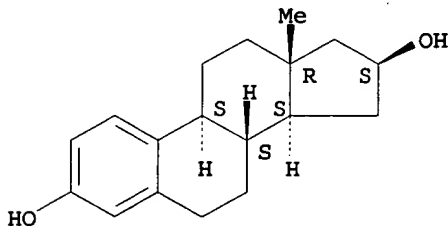
RL: PROC (Process)

(mitogenic action of, on uterus, mol. structure in relation to)

RN 1225-58-7 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, (16 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



CC 2-2 (Mammalian Hormones)

IT 50-27-1 50-28-2, Estradiol, biological studies 57-91-0,

17 α -Estradiol 547-81-9 552-80-7, Dimethylstilbestrol
 1090-04-6, 16 α -Estradiol 1225-58-7,
 16 β -Estradiol 1845-11-0, Nafoxidine 24643-97-8
 68047-06-3 71855-45-3, Indanestrol
 RL: PROC (Process)

(mitogenic action of, on uterus, mol. structure in relation to)

L52 ANSWER 3 OF 24 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1988:622771 HCAPLUS

DOCUMENT NUMBER: 109:222771

TITLE: Effect of endogenous and synthetic sex
steroids on the clearance of antibody-coated
cells

AUTHOR(S): Schreiber, A. D.; Nettle, F. M.; Sanders, M.
C.; King, M.; Szabolcs, P.; Friedman, D.;
Gomez, F.

CORPORATE SOURCE: Cancer Cent., Univ. Pennsylvania,
Philadelphia, PA, 19104, USA

SOURCE: Journal of Immunology (1988), 141(9), 2959-66
CODEN: JOIMA3; ISSN: 0022-1767

DOCUMENT TYPE: Journal

LANGUAGE: English

AB An exptl. model developed in the guinea pig, was used to study the effects of female sex hormones on macrophage clearance of IgG- and IgM-coated erythrocytes in the spleen and liver. Progesterone, its naturally occurring analog 17-hydroxyprogesterone, and its synthetic analog 16-methylprogesterone inhibited the clearance of IgG-coated erythrocytes by splenic macrophages. Furthermore, when splenic macrophages were isolated from progesterone-treated animals they expressed decreased Fc γ R activity. Estradiol, estriol, and the estrogen analog 1,3,5(10)-estratriene-3,16 β -diol enhanced splenic macrophage clearance of IgG-coated erythrocytes. This action of the estrogens could be partially inhibited by the antiestrogen tamoxifen. However, estradiol did not affect the C3-dependent clearance of IgM-coated erythrocytes by hepatic macrophages. Concurrent administration of estradiol and progesterone demonstrated that the action of estradiol was predominant. Thus, female sex hormones alter splenic macrophage Fc γ R function at concns. observed during the human menstrual cycle and pregnancy. This result may also explain alteration of disease activity in some human immunol. disorders during changes in the hormonal states.

IT 1225-58-7

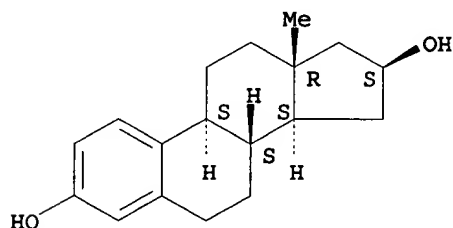
RL: BIOL (Biological study)

(IgG-coated erythrocyte clearance by spleen macrophage
stimulation by)

RN 1225-58-7 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, (16 β)- (9CI) (CA INDEX
NAME)

Absolute stereochemistry.



CC 2-4 (Mammalian Hormones)

Section cross-reference(s): 15

IT 50-27-1, Estriol 50-28-2, Estradiol, biological studies

1225-58-7

RL: BIOL (Biological study)
(IgG-coated erythrocyte clearance by spleen macrophage stimulation by)

L52 ANSWER 4 OF 24 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1987:96443 HCAPLUS

DOCUMENT NUMBER: 106:96443

TITLE: Influence of adrenergic receptors on ovarian progesterone secretion in the pseudopregnant cat and estradiol secretion in the estrous cat

AUTHOR(S): Wheeler, A. G.; Walker, M.; Lean, J.

CORPORATE SOURCE: Dep. Physiol. Pharmacol., Univ. Queensland, St. Lucia, 4067, Australia

SOURCE: Journal of Reproduction and Fertility (1987), 79(1), 195-205

CODEN: JRPFA4; ISSN: 0022-4251

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The infusion of isoprenaline [7683-59-2] or propranolol into the abdominal aorta of the pseudopregnant cat caused an increase or decrease, resp., in the ovarian progesterone [57-83-0] secretion rate. Apparently, the sympathetic innervation of the ovary has a physiol. influence on normal progesterone secretion, and this mechanism may explain stress-related increases in progesterone concns. The infusion of isoprenaline or propranolol after the stimulation of follicular growth had no consistent or convincing effect on estradiol [1225-58-7] secretion.

IT 1225-58-7

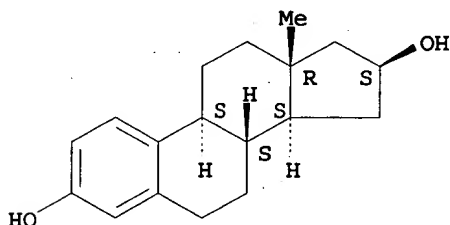
RL: PROC (Process)

(secretion of, by ovary, adrenergic receptors in relation to)

RN 1225-58-7 HCAPLUS

CN Estradiol, 1,3,5(10)-triene-3,16-diol, (16 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



CC 2-4 (Mammalian Hormones)

IT 1225-58-7

RL: PROC (Process)

(secretion of, by ovary, adrenergic receptors in relation to)

L52 ANSWER 5 OF 24 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1987:16187 HCAPLUS

DOCUMENT NUMBER: 106:16187

TITLE: Methylcholanthrene: a possible pseudosubstrate for adrenocortical 17 α -hydroxylase and aryl hydrocarbon hydroxylase

AUTHOR(S): Hornsby, Peter J.; Aldern, Kathy A.; Harris, Sandra E.

CORPORATE SOURCE: Sch. Med., Univ. California, La Jolla, CA, 92093, USA

SOURCE: Biochemical Pharmacology (1986), 35(19), 3209-19

CODEN: BCPCA6; ISSN: 0006-2952

DOCUMENT TYPE:

Journal

LANGUAGE:

English

AB In cultured bovine adrenocortical cells, the loss of steroid 17 α -hydroxylase (I) activity was observed after incubation with 3-methylcholanthrene (3-MC). The suppression of I by 3-MC was rapid (50% loss of activity in 10 h at 1 μ M 3-MC), did not exhibit a lag period, and was not affected by cycloheximide. Direct effects of 3-MC on I were observed only at high concns., but the concentration for 50% loss of activity was 0.3 μ M when 3-MC was added for 24 h prior to assay of I. High concns. (to 40 μ M) of substrate (progesterone), did not affect the loss of activity due to 3-MC. Loss of I activity was specific; steroid 11 β -hydroxylase was unaffected and cell growth was unaltered. However, 22-amino-23,24-bisnorchol-5-en-3 β -ol, an inhibitor of I, partially prevented the loss of I at 1-30 nM. 3-MC was thought to induce cytochrome P 450s via a receptor with high affinity for 2,3,7,8-tetrachlorodibenzo-p-dioxin (TCDD). TCDD was without effect on I over the range 10 nM-10 μ M. Benz[a]anthracene, 7,12-dimethylbenz[a]anthracene, benzo[a]pyrene, chrysene, and methylphenanthrenes suppressed I at high concns. (10-50 μ M for 50% loss of activity). Some steroids that lack a substituent at position 17 also caused loss of I. Like I, bovine adrenocortical cell aryl hydrocarbon hydroxylase (II) was found to be suppressed by exposure to 3-MC. Compds. that caused loss of I caused loss of II, with a similar order of potency and at similar concns. Suppression of II by 3-MC did not require protein synthesis and was prevented by an inhibitor of enzymic activity, α -naphthoflavone. This implied a degree of similarity of the cytochrome P 450s for I and II, but the activities were shown to be likely due to different enzymes. The suppression of I and II by 3-MC appeared not to occur by a receptor-mediated mechanism but to be similar to the suppression of steroid 11 β -hydroxylase and steroid 21-hydroxylase by steroid pseudosubstrates previously observed

IT 1225-58-7, Estra-1,3,5(10)-triene-3,16 β -diol

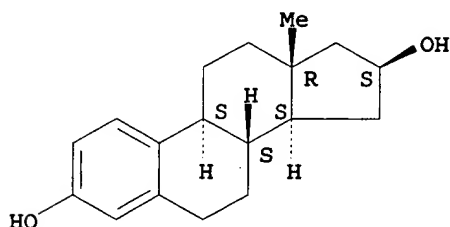
RL: BIOL (Biological study)

(aryl hydrocarbon hydroxylase and steroid 17 α -hydroxylase response to, in adrenocortical cells)

RN 1225-58-7 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, (16 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



CC 13-2 (Mammalian Biochemistry)

Section cross-reference(s): 7

IT 50-32-8, Benz[a]pyrene, biological studies 56-49-5,
 3-Methylcholanthrene 56-55-3, Benz[a]anthracene 57-97-6,
 7,12-Dimethylbenz[a]anthracene 63-05-8, Androstenedione
 218-01-9, Chrysene 832-69-9, 1-Methylphenanthrene 1153-51-1,
 5 α -Androst-16-en-3 α -ol 1225-58-7,
 Estra-1,3,5(10)-triene-3,16 β -diol 2531-84-2,
 2-Methylphenanthrene 7148-51-8, 5 α -Androst-16-en-3 β -
 ol 17012-89-4, 4-Methylcholanthrene 18339-16-7,

5 α -Androst-16-en-3-one

RL: BIOL (Biological study)

(aryl hydrocarbon hydroxylase and steroid 17 α -hydroxylase
response to, in adrenocortical cells)

L52 ANSWER 6 OF 24 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1985:574487 HCAPLUS

DOCUMENT NUMBER: 103:174487

TITLE: Isolation of novel microbial 3 α -,
3 β -, and 17 β -hydroxysteroid
dehydrogenases. Purification,
characterization, and analytical applications
of a 17 β -hydroxysteroid dehydrogenase
from an *Alcaligenes* sp.

AUTHOR(S): Payne, Donna W.; Talalay, Paul

CORPORATE SOURCE: Sch. Med., Johns Hopkins Univ., Baltimore, MD,
21205, USA

SOURCE: Journal of Biological Chemistry (1985),
260(25), 13648-55

CODEN: JBCHA3; ISSN: 0021-9258

DOCUMENT TYPE: Journal

LANGUAGE: English

AB By selecting for growth on testosterone or 17 β -estradiol as
the only source of organic C, a number of soil microorganisms which
contain highly active and novel, inducible, NAD-linked 3 α -,
3 β -, and 17 β -hydroxy steroid dehydrogenases were
isolated. Such enzymes are suitable for the microanal. of
steroids and of steroid-transforming enzymes, as well as for
performing stereoselective oxidns. and reduction of steroids. Of
particular interest among these organisms is a new species of
Alcaligenes containing 17 β -hydroxy steroid dehydrogenase (I)
easily separable from 3 β -hydroxy steroid dehydrogenase
activity. Unlike any of the other isolated organisms, this
Alcaligenes species contained no 3 α -hydroxy steroid
dehydrogenase activity. A large-scale purification (763-fold) to
homogeneity of the major induced I was achieved by ion-exchange,
hydrophobic, and affinity chromatogs. The enzyme has high
specific activity for the oxidation of testosterone (V_{max} = 303
 μ mol/min/mg protein; K_m = 3.6 μ M) and reacts almost equally
well with 17 β -estradiol (V_{max} = 356 μ mol/min/mg; K_m = 6.4
 μ M). It consists of apparently identical subunits mol. weight =
32,000 and exists in polymeric form under nondenaturing
conditions (mol. weight = 68,000 by gel filtration. and 86,000 by
polyacrylamide gel electrophoresis). The isoelec. point is pH
5.1. The enzyme is almost completely specific for
17 β -hydroxy steroids which may be Δ 5-olefins or ring A
phenols or have cis or trans A/B ring fusions. Substituents at
other positions are tolerated, although the presence of a
16 α - or 16 β -OH group blocks the oxidation of the
17 β -OH function. 3 β -Hydroxy steroids (A/B ring fusion
trans, but not cis, or Δ 5-olefins) are very poor substrates.
The application of this highly active, specific, and stable I to
the microestn. of steroids by enzymic cycling of nicotinamide
nucleotides and for the stereospecific oxidation of steroids is
demonstrated.

IT 1225-58-7

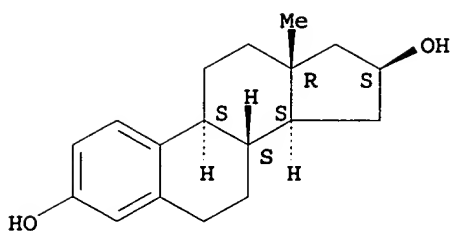
RL: BIOL (Biological study)

(17 β -hydroxy steroid dehydrogenase of *Alcaligenes*
specificity for, structure in relation to)

RN 1225-58-7 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, (16 β)- (9CI) (CA INDEX
NAME)

Absolute stereochemistry.



CC 7-2 (Enzymes)

Section cross-reference(s): 2, 9

IT 57-91-0 62-99-7 521-17-5 521-18-6 547-81-9 571-20-0
571-22-2 1156-92-9 1225-58-7 1816-85-9 1851-23-6
1852-53-5 2226-70-2 3066-12-4

RL: BIOL (Biological study)

(17β-hydroxy steroid dehydrogenase of *Alcaligenes*
specificity for, structure in relation to)

L52 ANSWER 7 OF 24 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1984:47664 HCAPLUS

DOCUMENT NUMBER: 100:47664

TITLE: Inhibitor specificity of the placental
microsomal oxidase system responsible for the
aromatization of epitestosterone
(17α-hydroxy-4-androsten-3-one)

AUTHOR(S): Sheean, Leon A.; Meigs, Robert A.

CORPORATE SOURCE: Sch. Med., Case Western Reserve Univ.,
Cleveland, OH, 44106, USA

SOURCE: Steroids (1983), 41(2), 225-41

CODEN: STEDAM; ISSN: 0039-128X

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Human placental microsomes converted epitestosterone to
17α-estradiol at rates of 23-48 pmol/min/mg protein with a
Km of 113 μM. The activity was inhibited 70-90% by concns. of
CO, metyrapone, octylamine, 7,8-benzoflavone, and 7-ethoxycoumarin
which had no effect on the aromatization of 4-androstene-3,17-
dione. Conversely, CN- and N3- were more effective inhibitors of
the conversion of the latter androgen. A variety of neutral
steroids inhibited the aromatization of epitestosterone with
19-norsteroids being particularly effective, but competitive
effects could not be demonstrated. Both 17β-hydroxy-4-estren-
3-one and 16α-hydroxy-4-androstene-3,17-dione caused a mixed
inhibition. A number of phenolic steroids were also inhibitory with
16-oxo compds. being particularly effective. Inhibition by
estrone was non-competitive (Ki = 16 μM). The aromatization of
epitestosterone resembles placental microsomal oxidase activities
against estrone and benzo[a]pyrene in its inhibitor specificity
and epitestosterone may be the native substrate for an oxidase
also active in the metabolism of aromatic xenobiotic chems.

IT 1225-58-7

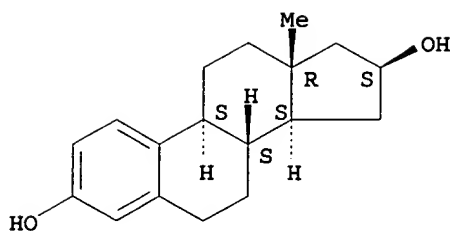
RL: BIOL (Biological study)

(epitestosterone oxidase of human placenta microsomes
inhibition by)

RN 1225-58-7 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, (16β)- (9CI) (CA INDEX
NAME)

Absolute stereochemistry.



CC 7-3 (Enzymes)

IT 50-27-1 50-28-2, biological studies 53-16-7, biological
 studies 53-45-2 53-63-4 56-53-1 57-91-0 58-18-4
 58-22-0 63-01-4 63-02-5 63-05-8 362-06-1 434-03-7
 434-22-0 521-18-6 547-81-9 566-75-6 566-76-7 571-52-8
 734-32-7 793-89-5 846-46-8 1089-78-7 1090-04-6
 1225-58-7 1228-72-4 1228-73-5 1624-62-0 1743-60-8
 3601-97-6 3646-30-8 3962-66-1 4011-48-7 6038-23-9
 6132-10-1 6199-65-1

RL: BIOL (Biological study)

(epitestosterone oxidase of human placenta microsomes
 inhibition by)

L52 ANSWER 8 OF 24 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1981:561659 HCAPLUS

DOCUMENT NUMBER: 95:161659

TITLE: Characteristics of membrane transport of
 methotrexate by cultured human breast cancer
 cells

AUTHOR(S): Schilsky, Richard L.; Bailey, Brenda D.;
 Chabner, Bruce A.

CORPORATE SOURCE: Div. Cancer Treat., Natl. Cancer Inst.,
 Bethesda, MD, 20205, USA

SOURCE: Biochemical Pharmacology (1981), 30(12),
 1537-42

CODEN: BCPCA6; ISSN: 0006-2952

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Methotrexate (I) [59-05-2] transport by MCF-7 cells and cultured
 estrogen- and insulin [9004-10-8]-sensitive human breast cancer
 cells exhibited a high-affinity carrier system that displayed
 Michaelis-Menten kinetics (K_m 8.22 μ M, V_{max} 12.22 nmol/min/g
 cell protein), was competitively inhibited by leucovorin and
 aminopterin but not folic acid, and was temperature-sensitive (Q_{10}
 2.25). Initial uptake rates were not affected by ouabain or NaN_3 ,
 but efflux of intracellular drug was markedly inhibited by NaN_3 ,
 suggesting an energy-dependent efflux mechanism. A low affinity
 uptake component was identified with extracellular $I > 10 \mu$ M,
 possibly representing a lower affinity membrane carrier or passive
 diffusion. Growth of MCF-7 cells in serum-free medium induced an
 increase in K_m to 15.93 μ M; insulin, but not estradiol, reversed
 this change. Thus, I transport in this human solid tumor is
 similar to that in human leukemia cells.

IT 1225-58-7

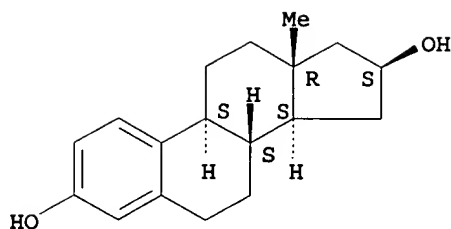
RL: BIOL (Biological study)

(methotrexate transport by breast cancer cells response to)

RN 1225-58-7 HCAPLUS

CN Estradiol, 1,3,5(10)-triene-3,16-diol, (16 β)- (9CI) (CA INDEX
 NAME)

Absolute stereochemistry.



CC 1-2 (Pharmacodynamics)

IT 1225-58-7 9004-10-8, biological studies

RL: BIOL (Biological study)

(methotrexate transport by breast cancer cells response to)

L52 ANSWER 9 OF 24 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1978:116912 HCAPLUS

DOCUMENT NUMBER: 88:116912

TITLE: Inhibition of human placental
17 β -hydroxysteroid dehydrogenase by
steroids and nonsteroidal alcohols: aspects
of inhibitor structure and binding specificity

AUTHOR(S): Blomquist, Charles H.; Kotts, Claire E.;
Hakanson, Erick Y.

CORPORATE SOURCE: Dep. Obstet. Gynecol., St. Paul-Ramsey Hosp.,
St. Paul, MN, USA

SOURCE: Archives of Biochemistry and Biophysics
(1978), 186(1), 35-41

CODEN: ABBIA4; ISSN: 0003-9861

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Inhibition of human placental 17 β -hydroxysteroid
dehydrogenase by C18 and C19 steroids and nonsteroidal alcs. was
assayed at pH 9.0 with 17 β -estradiol 3-Me ether and NAD as
reactants. The nonsteroidal alcs. tested were poor inhibitors.
Cyclopentanol and cyclohexanol had K_i values >5 mM. Nonarom. C18
and C19 steroids with O functions at both positions 3 and 17 gave
no detectable inhibition or had K_i values ≥ 160 μ M.
3 β -Hydroxy-5,16-androstadiene, 5-androsten-3 β -ol,
1,3,5(10)-estratrien-3-ol, and 1,3,5(10),16-estratetraen-3-ol,
steroids lacking a C(17) oxygen function, had K_i values of 1.8,
6.0, 0.04, and 0.17 μ M, resp., demonstrating that both C18 and
C19 steroids can bind at the steroid site. Binding specificity is
narrowed and binding affinity for nonarom. steroids weakened by O
functions at C(17) or both C(3) and C(17). The structural
implications of the specificity data for steroid recognition and
complex formation and in vivo control of enzyme activity are
discussed.

IT 1225-58-7

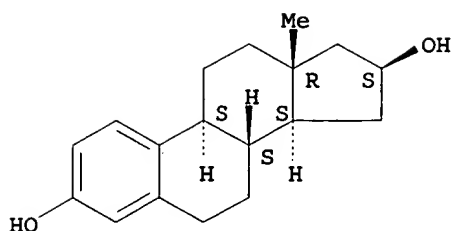
RL: BIOL (Biological study)

(17 β -hydroxysteroid dehydrogenase inhibition by, kinetics
of)

RN 1225-58-7 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, (16 β)- (9CI) (CA INDEX
NAME)

Absolute stereochemistry.



CC 7-3 (Enzymes)

IT 50-27-1 53-16-7, biological studies 53-43-0 53-63-4
 57-91-0 58-22-0 63-05-8 96-41-3 100-51-6, biological
 studies 108-93-0, biological studies 108-95-2, biological
 studies 112-47-0 547-81-9 1150-90-9 1224-94-8
 1225-58-7 1476-64-8 1912-63-6 3646-28-4 3937-56-2
 5088-64-2 54200-08-7

RL: BIOL (Biological study)

(17 β -hydroxysteroid dehydrogenase inhibition by, kinetics
 of)

L52 ANSWER 10 OF 24 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1973:505459 HCAPLUS

DOCUMENT NUMBER: 79:105459

TITLE: Chromogenic reactions of steroids with strong acids. IV. Specificity of the Kober reaction

AUTHOR(S): Kimura, Michiya; Kawata, Meiji; Akiyama,
 Kazuyuki; Harita, Kazuaki; Miura, Toshiaki
 CORPORATE SOURCE: Fac. Pharm. Sci., Hokkaido Univ., Sapporo,
 Japan

SOURCE: Chemical & Pharmaceutical Bulletin (1973),
 21(8), 1720-6

CODEN: CPBTAL; ISSN: 0009-2363

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The structural requirements were investigated for the Kober
 reaction of steroidal mols. On the basis of the data given by 94
 phenolic steroids and related substance, a compound will give the
 pos. Kober reaction when a steroidal ring system, a phenolic ring
 A, double bond or O function in ring D, an angular Me group at
 C-13, and an angular H atom are present in its mol.

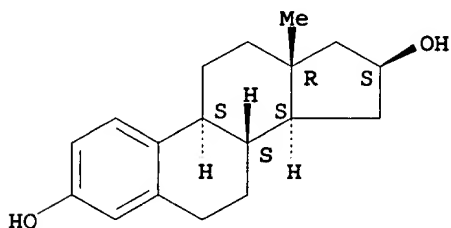
IT 1225-58-7

RL: RCT (Reactant); RACT (Reactant or reagent)
 (Kober reaction of, absorption spectra and)

RN 1225-58-7 HCAPLUS

CN Estradiol, 1,3,5(10)-triene-3,16-diol, (16 β)- (9CI) (CA INDEX
 NAME)

Absolute stereochemistry.



CC 32-3 (Steroids)

Section cross-reference(s): 22

IT 50-23-7 50-24-8 53-41-8 53-42-9 53-45-2 57-83-0,

reactions	57-88-5, reactions	58-22-0	72-33-3	145-13-1
362-06-1	362-07-2	434-22-0	481-29-8	482-49-5
517-07-7	517-09-9	521-10-8	521-11-9	521-17-5
604-82-0	846-46-8	901-93-9	960-28-1	966-47-2
1089-80-1	1217-09-0	1225-58-7	1228-73-5	1232-80-0
1239-35-6	1616-20-2	1730-48-9	2208-13-1	2259-89-4
3601-97-6	4011-48-7	4147-12-0	4954-14-7	5764-23-8
5976-64-7	5976-65-8	5976-68-1	5976-70-5	5982-51-4
6714-06-3	7291-41-0	10323-17-8	13251-78-0	14550-57-3
15236-73-4	15292-90-7	16127-98-3	19518-61-7	26584-88-3
26584-89-4	26584-90-7	28336-31-4	31019-01-9	35456-73-6
40822-17-1	50394-23-5	50394-95-1	50395-01-2	50395-07-8
50395-10-3	50395-12-5	50395-16-9	50395-18-1	50395-21-6
50395-26-1	50395-28-3	50395-30-7	50395-31-8	50395-34-1
50395-35-2	50395-38-5	50770-19-9		

RL: RCT (Reactant); RACT (Reactant or reagent)
(Kober reaction of, absorption spectra and)

L52 ANSWER 11 OF 24 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1970:495274 HCAPLUS

DOCUMENT NUMBER: 73:95274

TITLE: Absorption and fluorescence spectra of phenolic steroids and their Kober chromophore

AUTHOR(S): De Lauzon, Solange

CORPORATE SOURCE: Lab. Chim. Biol., Fac. Med., Paris, Fr.

SOURCE: Bulletin de la Societe de Chimie Biologique (1970), 52(2), 181-209

CODEN: BSCIA3; ISSN: 0037-9042

DOCUMENT TYPE: Journal

LANGUAGE: French

AB A complete assignment was made of the absorption and fluorescence spectra of a number of phenolic steroids and their derivs. and the results may be used to identify and determine each estrogen studied. The reaction of various derivs. which cannot be differentiated by the behavior of the Kober chromophore, or do not form a Kober chromophore, in H₂SO₄ and H₃PO₄ was used as an identification method. These derivs. included ketonic derivs. of estrone and estradiol, 16-hydroxy derivs. of estrone and their Et and Me ethers, and non-oxygenated C₁₇ derivs. The Kober reaction was used as a determination method for derivs. giving a characteristic absorption maximum, and the Ittrich modification allowed a sensitive anal. method to be developed for the steroid groups.

IT 1225-58-7

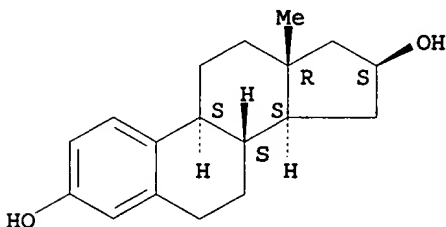
RL: PRP (Properties)

(fluorescence and visible spectra of, and its Kober chromogen)

RN 1225-58-7 HCAPLUS

CN Estr-1,3,5(10)-triene-3,16-diol, (16 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



CC 6 (Biochemical Methods)

IT 50-27-1 50-28-2, properties 53-16-7, properties 57-91-0

362-07-2 362-08-3 547-81-9 566-75-6 566-76-7 571-92-6

793-89-5 966-06-3 1035-77-4 1090-04-6 1225-58-7

1228-72-4 1228-73-5 1229-33-0 1474-50-6 1474-53-9
 1476-34-2 1624-62-0 3434-76-2 3434-77-3 3434-78-4
 3434-79-5 3434-81-9 5976-64-7 6038-22-8 7004-98-0
 24721-15-1 26849-20-7 28872-65-3

RL: PRP (Properties)

(fluorescence and visible spectra of, and its Kober chromogen)

L52 ANSWER 12 OF 24 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1970:452631 HCAPLUS

DOCUMENT NUMBER: 73:52631

TITLE: Steroid utilization by amphibian skin

AUTHOR(S): Ferguson, M. M.; McGadey, J.

CORPORATE SOURCE: Anat. Dep., Univ. Glasgow, Glasgow, UK

SOURCE: Histochemie (1970), 22(1), 36-8

CODEN: HICHAU; ISSN: 0018-2222

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The glands which secrete unpleasant tasting or toxic substances in amphibian dermis were investigated histochem. for hydroxysteroid dehydrogenase (I) activity to draw comparisons with mammalian sebaceous glands, which are known to utilize hydroxy steroids. Skin sections from frogs were incubated with 15 different steroids; serial sections were also stained with hematoxylin and eosin and by the periodic acid-Schiff (PAS) reaction to differentiate mucous glands. The frog skin contained at least 2 functional types of glands; one type was PAS-pos., while the second type, less common, was PAS-neg. but exhibited intense I activity. Tissue incubated with pregnenolone, dehydroepiandrosterone, 3β -hydroxyandrost-5-en-16-one 3-methyl ether, and 2β -hydroxyprogesterone exhibited no formazan deposits.

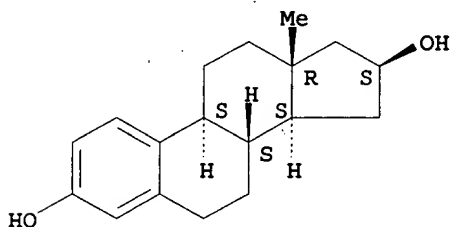
IT 1225-58-7

RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process) (metabolism of, by skin)

RN 1225-58-7 HCAPLUS

CN Estr-1,3,5(10)-triene-3,16-diol, (16 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



CC 4 (Hormones and Related Substances)

IT 50-23-7, biological studies 50-28-2, biological studies
 53-06-5, biological studies 53-41-8 53-42-9 53-43-0,
 biological studies 58-22-0, biological studies 145-13-1
 145-15-3 481-29-8 571-31-3 1225-58-7 5888-04-0
 6038-34-2

RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process) (metabolism of, by skin)

L52 ANSWER 13 OF 24 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1965:10380 HCAPLUS

DOCUMENT NUMBER: 62:10380

ORIGINAL REFERENCE NO.: 62:1938e-f

TITLE: A search for inhibitors of prostate growth stimulators
 AUTHOR(S): Tesar, Charles; Scott, William Wallace
 CORPORATE SOURCE: Johns Hopkins Hosp., Baltimore, MD, USA
 SOURCE: Investigative Urology (1964), 1(5), 482-98
 CODEN: INURAQ; ISSN: 0021-0005

DOCUMENT TYPE: Journal
 LANGUAGE: English

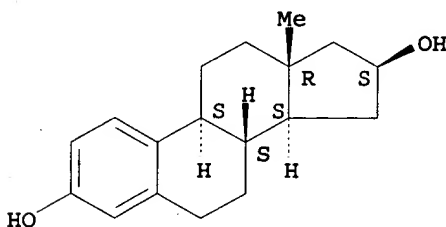
AB Wistar rats received 0.4 mg. testosterone propionate (I) s.c. every other day for 8 days following castration. Test compds. were given at 0.5, 1, and 2 mg. every other day for 7 days, with or without 0.4 mg. I in castrate and noncastrates, resp. Within 48 h. of the 7th (final) injection, animals were sacrificed with CHCl₃, and the prostate weight to body weight ratio, and the prostate weight index were determined. The greatest prostate growth inhibitor was 17 β -estradiol, and some weak inhibition was seen with 6 α -methyl-4-pregnene-3,20-dione-17 α -ol acetate, androstane-3,17-dione, and 2 α -methyl-4-estrene-17 β -ol-3-one, the inhibitory effect being seen only in intact rats, and not in castrates, for all 52 compds. tested.

IT 1225-58-7, Estra-1,3,5(10)-triene-3,16 β -diol
 (as prostate growth inhibitor)

RN 1225-58-7 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, (16 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



CC 58 (Hormones)

IT 57-91-0, 17 α -Estradiol 65-14-5, Valeronitrile,
 2,3-bis(p-hydroxyphenyl)- 68-22-4, 19-Nor-17 α -pregn-4-en-
 20-yn-3-one, 17-hydroxy- 68-96-2, Pregn-4-ene-3,20-dione,
 17-hydroxy- 71-58-9, Pregn-4-ene-3,20-dione,
 17-hydroxy-6 α -methyl-, acetate 521-12-0,
 5 α -Androstan-3-one, 17 β -hydroxy-2 α -methyl-,
 propionate 571-22-2, 5 β -Androstan-3-one, 17 β -hydroxy-
 1039-17-4, Androsta-4,9(11)-dien-3-one, 17 β -hydroxy-17-methyl-
 1090-04-6, Estra-1,3,5(10)-triene-3,16 α -diol 1092-04-2,
 Estr-4-en-3-one, 17 β -hydroxy-2 α -methyl- 1093-46-5,
 19-Nor-17 α -pregn-20-yne-3 β ,17-diol 1094-07-1,
 Estra-1,3,5(10)-triene-17-one, 3-hydroxy-1,2-dimethyl- 1096-38-4,
 Pregna-4,16-diene-3,20-dione 1225-58-7,
 Estra-1,3,5(10)-triene-3,16 β -diol 1229-33-0,
 Estra-1,3,5(10)-triene-16 β -ol, 3-methoxy- 1428-66-6, Acetic
 acid, [(17-oxoestra-1,3,5(10)-triene-3-yl)oxy]- 1428-67-7,
 Propionitrile, 2,3-bis(p-hydroxyphenyl)- 5717-79-3,
 5 α -Androstane-3,17-dione, 17-oxime 6808-29-3,
 19-Nor-17 α -pregn-20-yn-3-one, 17-hydroxy-
 (as prostate growth inhibitor)

L52 ANSWER 14 OF 24 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1960:98911 HCAPLUS

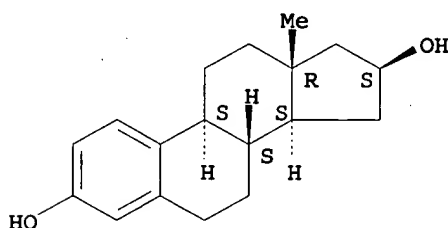
DOCUMENT NUMBER: 54:98911

ORIGINAL REFERENCE NO.: 54:18799c-d

TITLE: Cytostatic activities of steroidal estrogens

against zebra-fish embryos
 AUTHOR(S): Jones, Roy W.; Rhone, James R.; Huffman, Max N.
 CORPORATE SOURCE: Oklahoma State Univ., Stillwater
 SOURCE: Proceedings of the Society for Experimental Biology and Medicine (1960), 104, 190-1
 CODEN: PSEBAA; ISSN: 0037-9727
 DOCUMENT TYPE: Journal
 LANGUAGE: Unavailable
 AB cf. CA 52, 3171c. The cytostatic effects of 14 steroidal estrogens (named) and the 3-Me and 3-Et ethers of each were tested on embryos of zebra-fish (*Brachydanio rerio*) as test object. Many were inactive in the concns. used. Most active was 17-dihydro-17 β -equilin 3-ethyl ether (effective at 0.5 p.p.m.). There was no relation whatever between estrogenic hormone potency and cytostatic potency.
 IT 1225-58-7, Estra-1,3,5(10)-triene-3,16 β -diol (as cell-division inhibitor)
 RN 1225-58-7 HCAPLUS
 CN Estra-1,3,5(10)-triene-3,16-diol, (16 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



CC 11I (Biological Chemistry: Zoology)
 IT 50-28-2, Estradiol 57-91-0, 17 α -Estradiol 517-09-9,
 Equilenin 1035-77-4, Estra-1,3,5(10)-trien-17 β -ol,
 3-methoxy- 1090-04-6, Estra-1,3,5(10)-triene-3,16 α -diol
 1225-58-7, Estra-1,3,5(10)-triene-3,16 β -diol
 1229-33-0, Estra-1,3,5(10)-trien-16 β -ol, 3-methoxy-
 1423-97-8, Estra-1,3,5(10),6,8-pentaene-3,17 β -diol
 1474-50-6, Estra-1,3,5(10)-trien-17-one, 3-ethoxy- 1624-62-0,
 Estra-1,3,5(10)-trien-17-one, 3-methoxy- 3494-09-5,
 Estra-1,3,5(10)-trien-17 β -ol, 3-ethoxy- 3563-27-7,
 Estra-1,3,5(10),7-tetraene-3,17 β -diol 4820-55-7,
 Estra-1,3,5(10),6,8-pentaen-17 β -ol, 3-methoxy- 6030-83-7,
 Estra-1,3,5(10),7-tetraen-17-one, 3-methoxy- 6038-22-8,
 Estra-1,3,5(10)-trien-16-one, 3-methoxy- 13587-68-3,
 Estra-1,3,5(10),7-tetraen-17 β -ol, 3-methoxy- 58031-57-5,
 Estra-1,3,5(10),6,8-pentaen-17 β -ol, 3-ethoxy- 102168-54-7,
 Estra-1,3,5(10)-triene-16,17-dione, 3-ethoxy- 110145-73-8,
 Estra-1,3,5(10),7-tetraen-17-one, 3-ethoxy- 110876-82-9,
 Estra-1,3,5(10),7-tetraen-17 β -ol, 3-ethoxy- 112949-05-0,
 Estra-1,3,5(10)-trien-16 β -ol, 3-ethoxy-
 (as cell-division inhibitor)

L52 ANSWER 15 OF 24 HCAPLUS COPYRIGHT 2006 ACS on STN

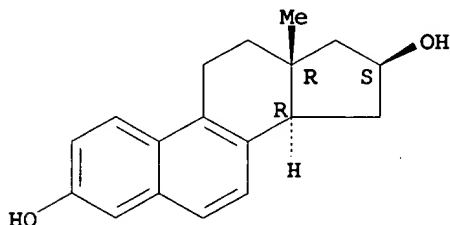
ACCESSION NUMBER: 1960:74827 HCAPLUS
 DOCUMENT NUMBER: 54:74827
 ORIGINAL REFERENCE NO.: 54:14309a-e
 TITLE: 16 α -Hydroxysteroids
 PATENT ASSIGNEE(S): Nepera Chemical Co., Inc.
 DOCUMENT TYPE: Patent
 LANGUAGE: Unavailable
 FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 823955		19591118	GB 1956-11714	1956 0417

- AB The title compds., their ethers and esters were prepared by heating an arenesulfonate of the corresponding 16 β -ol with an alkali metal lower alkanolate in the corresponding alkanolic acid and saponifying the resulting 16 α -acylate. Thus, 4.4 g. p-MeC₆H₄SO₂Cl added to a solution of 1 g. 1,3,5(10)-estratriene-3,16 β -diol in 28 ml. dry C₅H₅N at 0°, the mixture kept 2 days, diluted with ice H₂O containing 10% NaCl, left 24 hrs. at 5°, extracted with Et₂O, the exts. washed, the washings extracted with Et₂O and the combined exts. evaporated gave 1.9 g. crude 3,16 β -ditosylate, which refluxed 1 hr. with 4.8 g. fused NaOAc in 92 ml. AcOH, the mixture cooled and diluted with ice H₂O containing 10% NaCl, after 24 hrs. the precipitate separated, dried and refluxed 1 hr. with 60 ml. 2.5N KOH in 200 ml. MeOH, the MeOH distilled, 100 ml. H₂O, then 10 ml. concentrated HCl added, the pH adjusted to 5-6, the precipitate separated, dried at 40° and crystallized from Me₂CO-hexane then aqueous MeOH gave 0.55 g. 3,16 α -estradiol (I), m. 213-15°, raised to 224-4.5°, [α]_{25D} 85° (c 0.76, 95% EtOH), after purification via its 3,16 α -diacetate, m. 116-17°. Benzoylation of I in 0.5N NaOH gave the 3-monobenzoate, m. 179.5-81.0°; benzoylation in C₅H₅N gave the 3,16-dibenzoate, m. 130.5-1.5°. Similarly, 118 mg. 3-methoxyestra-1,3,5(10)-trien-16 β -ol gave 38 mg. estradiol 16 α -acetate 3-methyl ether, m. 123-3.5°; 575 mg. androstan-3 β -ol-16-one dissolved in 300 ml. refluxing MeOH, cooled, 0.39 g. NaBH₄ added, the solution swirled 1 hr., 4 ml. 50% AcOH added, the solution concentrated to 100 ml. and 100 ml. ice H₂O added yielded 550 mg. 3 β -benzoyloxyandrostan-16 β -ol (II), m. 168-9°; 400 mg. II epimerized as above gave androstane-3 β ,16 α -diol, m. 187.5-88°, [α]_{25D} -4° (c 0.777, 95% EtOH), which with Ac₂O in C₅H₅N gave the diacetate, m. 174-4.5° [α]_{23D} -26° (c 0.963, CHCl₃). Other starting materials are equilinen-16-one and 5-isoandrosterone. I displays considerable estrogenic activity, in contrast to its 16 β epimer.
- IT 110012-46-9, Estra-1,3,5(10),6,8-pentaene-3,16 β -diol (isomerization of)
- RN 110012-46-9 HCAPLUS
- CN Estra-1,3,5(10),6,8-pentaene-3,16-diol, (16 β) - (9CI) (CA INDEX NAME)

Absolute stereochemistry.



- CC 10J (Organic Chemistry: Steroids)
- IT 109581-80-8, Estra-1,3,5(10),7-tetraene-3,16 β -diol
110012-46-9, Estra-1,3,5(10),6,8-pentaene-3,16 β -diol (isomerization of)

L52 ANSWER 16 OF 24 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1959:17432 HCAPLUS

DOCUMENT NUMBER: 53:17432

ORIGINAL REFERENCE NO.: 53:3276g-i,3277a-f

TITLE: Synthesis of 1,3,5(10)-estratriene-3,16 β ,17 α -triol

AUTHOR(S): Fishman, Jack; Biggerstaff, Warren R.

CORPORATE SOURCE: Sloan-Kettering Inst. for Cancer Research, New York, NY

SOURCE: Journal of Organic Chemistry (1958), 23, 1190-2

CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

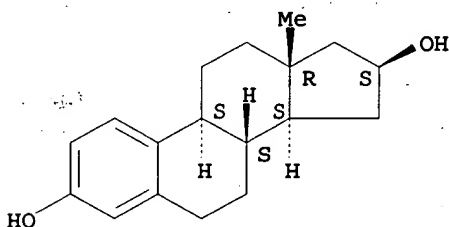
OTHER SOURCE(S): CASREACT 53:17432

AB Preparation of 1,3,5(10)-estratriene-3,16 β ,17 α -triol (I) is described. The 16 α - (II) and 16 α -bromo epimers (III) of estrone were also prepared and some of their reactions studied. Of the 4 possible estriols isomeric at C-16 and C-17 only 3 are known. The present authors undertook the preparation of the remaining isomer, I. Estrone enol diacetate (1 g.) in CCl₄ containing some K₂CO₃ was treated with 1 equivalent of Br in CCl₄ and the mixture worked up to give 700 mg. 16 α -bromoestrone acetate (IV), m. 169-71° (MeOH), [α]_D²⁵ 119° (CHCl₃). IV (0.3 g.) in 4% alc. H₂SO₄ left 20 hrs. at room temperature, diluted with H₂O, and extracted with CHCl₃ gave 243 mg. II, needles, m. 225-8° (C₆H₆), [α]_D²⁵ 120° (CHCl₃). Acetylation of II with Ac₂O and C₅H₅N regenerated IV. IV (0.5 g.) in a min. amount of 1:1 C₆H₆-ligroine was absorbed on Al₂O₃, left overnight on the column and eluted with first 3:2 and then 4:1 C₆H₆-ligroine, and the fractions combined on the basis of m.p. The first 5 fractions gave on crystallization 0.23 g. pure IV. Fractions 6-10 were mixts., and fractions 10-14 gave 47 mg. 16 β -bromoestrone acetate (V), needles, m. 170-3° (MeOH), [α]_D²⁵ 156° (CHCl₃). Subsequent fractions eluted from the column with more polar solvents proved to be a mixture of the hydrolyzed II and III. A mixed m.p. of V with IV showed a depression of 40°; the infrared spectra of II and III in CS₂ were different in the 1400-650 cm.⁻¹, but there was no difference in the position of the CO band at 1758 cm.⁻¹ Paper chromatography in several systems failed to sep. the 2 isomers. Room temperature hydrolysis of V 20 hrs. with 4% alc. H₂SO₄ gave free III, needles, m. 224-7° (sublimation) (C₆H₆). An analytical sample of III m. 225-8°, [α]_D²⁵ 154° (CHCl₃). III could be obtained by refluxing IV with 4% alc. H₂SO₄ overnight; the resultant mixture was predominantly III which was purified by fractional crystallization. Acetylation of III gave V. IV (1 g.) stirred 2 hrs. at 0° with excess LiAlH₄ in anhydrous Et₂O, the excess reagent destroyed with H₂O and acidified with dilute HCl, and the organic phase evaporated gave 0.78 g. gum. Without purification, the material refluxed 4 hrs. with 5% alc. KOH, diluted with H₂O, extracted with CHCl₃, and chromatographed on Al₂O₃ gave 0.24 g. 16 β ,17 β -epoxy-1,3,5(10)-estratrien-3-ol (VI), m. 200-4° (C₆H₆-ligroine), [α]_D²⁵ 119° (CHCl₃), and 92 mg. estrone. The structure of VI was established by reduction with LiAlH₄ to give 16 β -estradiol (VII), identical with a specimen prepared from 1,3,5(10)-estratrien-16-one by NaBH₄ reduction. VII m. 224-6°. V (150 mg.) reduced under identical conditions with LiAlH₄ followed by heating with alkali gave 94 mg. estrone. No 16 α ,17 α -oxide was isolated. VI (0.3 g.) in 30 cc. AcOH refluxed 4 hrs., evaporated, refluxed 1.5 hrs. with 6% alc. KOH, diluted, acidified, and extracted with CHCl₃ gave 0.3 g. solid which was chromatographed on Al₂O₃ to give 124 mg. I, m. 248-50° (C₆H₆-MeOH), [α]_D²⁵ 61° (alc.). The subsequent fractions eluted weighed 64 mg. and proved to be

the other trans isomer, 1,3,5(10)-estratriene-3,16 β ,17 α -triol (VIII). The infrared spectrum of I in KBr showed differences from the other 3 estriol isomers. Paper chromatography in C₆H₆-MeOH-H₂O-EtOAc system separated I from its isomers. I was less polar than VIII but considerably more polar than the 2 cis triols in the solvent system used. 1,3,5(10),16-Estratetraen-3-ol benzoate (100 mg.), m. 161-6°, in Et₂O treated with BzO₂H gave 111 mg. crude 16 α ,17 α -epoxy-1,3,5(10)-estratrien-3-ol benzoate. Without further purification this material was refluxed 2 hrs. with 3 cc. AcOH under N, the AcOH removed, and the residue refluxed 1.5 hrs. in 8% alc. KOH to give 73 mg. yellow solid, which, decolorized and crystallized, gave 23 mg. solid which was chromatographed on silica to give 12 mg. I. These results confirm the assignment of the Br orientation in II and III and also support the previous finding (C.A. 52, 5445b) that a 16 β -substituent results in the stereospecific β -reduction of the 17-one while a 16 α -substituent makes the reduction only stereoselective, with about 10-15% of α -reduction. The pharmacol. effects are being investigated.

IT 1225-58-7, Estra-1,3,5(10)(triene-3,16 β -diol
(preparation of)
RN 1225-58-7 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, (16 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



CC 10J (Organic Chemistry: Steroids)
IT 50-27-1, Estriol 472-57-1, Estra-1,3,5(10)-trien-3-ol,
16 β ,17 β -epoxy- 793-89-5, Estra-1,3,5(10)-triene-
3,16 β ,17 α -triol 1225-58-7,
Estra-1,3,5(10)(triene-3,16 β -diol 1228-71-3, Estrone,
16 β -bromo- 1239-35-6, Estrone, 16 α -bromo-, acetates
65912-80-3, Estrone, 16 β -bromo-, acetates 71765-95-2,
Estrone, 16 α -bromo- 114277-40-6, Estra-1,3,5(10)-trien-3-
ol, 16 α ,17 α -epoxy-, benzoate
(preparation of)

L52 ANSWER 17 OF 24 HCAPLUS COPYRIGHT 2006 ACS on STN

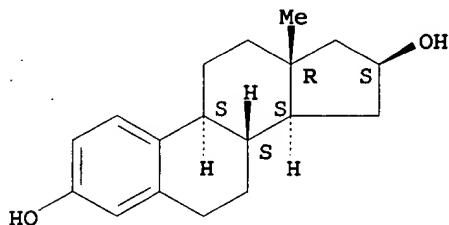
ACCESSION NUMBER: 1958:93818 HCAPLUS
DOCUMENT NUMBER: 52:93818
ORIGINAL REFERENCE NO.: 52:16548d-f
TITLE: Comparative ability of some steroids and their
esters to enhance the renal
 β -glucuronidase activity of mice
AUTHOR(S): Fishman, Wm. H.; Lipkind, J. B.
CORPORATE SOURCE: Tufts Univ. School of Med., Boston, MA
SOURCE: Journal of Biological Chemistry (1958), 232,
729-36
CODEN: JBCHA3; ISSN: 0021-9258
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB cf. C.A. 50, 17081h. The mouse renal β -glucuronidase
response permits a more reliable estimate of the potency of

testosterone esters. A dose-response curve in which greatly reduced amts. of steroid were used was employed. The potency of a steroid in eliciting the β -glucuronidase response is defined as 24 times the reciprocal of the dose required to produce a kidney assaying 10,000 units/g. The standard of reference is testosterone. According to this measure, testosterone propionate shows a potency of 60 and that of testosterone is 3.0. Nortestosterone cyclopentylpropionate was the most potent compound (potency 150). There is a marked difference in response between testosterone propionate and its other esters vs. testosterone. 3,16 β -Estradiol and 16-oxoestrone gave 2- to 3-fold increases in renal β -glucuronidase. The introduction of a 17-Me or 17-Et group into nortestosterone increased its potency as determined by the renal β -glucuronidase response.

IT 1225-58-7, Estra-1,3,5(10) (triene-3,16 β -diol
(potentiation of β -glucuronidase of kidneys by)
RN 1225-58-7 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, (16 β)- (9CI) (CA INDEX
NAME)

Absolute stereochemistry.



CC 11F (Biological Chemistry: Physiology)
IT 601-63-8, Estr-4-en-3-one, 17 β -hydroxy-,
cyclopentanepropionate 1225-58-7, Estra-1,3,5(10) (triene-
3,16 β -diol 1228-73-5, Estra-1,3,5(10)-triene-16,17-dione,
3-hydroxy- 100151-63-1, Estr-4-en-3-one, 17 β -hydroxymethyl-
(potentiation of β -glucuronidase of kidneys by)

L52 ANSWER 18 OF 24 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1957:101244 HCAPLUS

DOCUMENT NUMBER: 51:101244

ORIGINAL REFERENCE NO.: 51:18311d-g

TITLE: The effect of natural and synthetic estrogens
on reticuloendothelial system function

AUTHOR(S): Heller, J. H.; Meier, R. M.; Zucker, R.; Mast,
G. W.

CORPORATE SOURCE: New England Inst. for Med. Research,
Ridgefield, CT

SOURCE: Endocrinology (1957), 61, 235-41

DOCUMENT TYPE: Journal

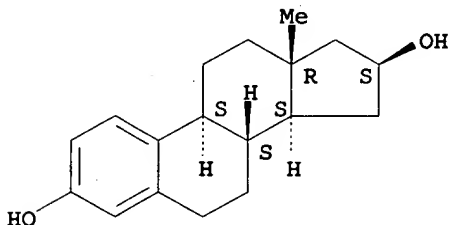
LANGUAGE: Unavailable

AB The activity of the reticuloendothelial system was determined by measuring the rate of disappearance by phagocytosis of intravenously injected colloidal C from the blood. The colloid uptake of various organs was determined by assaying for CrP32O4 content after an intravenous injection. Steroids increasing phagocytic velocity 100% or more were: estradiol, ethynylestradiol, estradiol-16-one, 1,3,5-estratriene-3,16 β -diol, 3-methoxy-1,3,5-estratriene-16 β -ol, estriol, 16-epiestriol, 3-methoxy-1,3,5-estratriene-16 β ,17 β -diol, and 3-ethoxy-1,3,5-estratriene-16 β ,17 β -diol; inactive were: 5-androstene-3 β ,16 β -diol, androstane-3,16 β -diol, androstane-3 α -ol-16-one, 4-androstene-3,16-dione, 5-androstene-3 β -ol-16-one, 3 β -methoxy-5-androstene-16-

one, 1,3,5-estratriene-3,6 α -diol, and 3-methoxy-1,3,5-estratriene-16-one. Stimulated activity of the reticuloendothelial system was accompanied by liver and spleen enlargement, without however, much increase in total colloid uptake by these organs.

IT 1225-58-7, Estra-1,3,5(10)-triene-3,16 β -diol
(effect on reticuloendothelial system)
RN 1225-58-7 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, (16 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



CC 11H (Biological Chemistry: Pharmacology)
IT 566-75-6, Estra-1,3,5(10)-triene-16-one, 3,17 β -dihydroxy-
1225-58-7, Estra-1,3,5(10)-triene-3,16 β -diol
1229-33-0, Estra-1,3,5(10)-triene-16 β -ol, 3-methoxy-
3434-79-5, Estra-1,3,5(10)-triene-16 β ,17 β -diol,
3-methoxy- 26849-20-7, Estra-1,3,5(10)-triene-16 β ,17 β -
diol, 3-ethoxy-
(effect on reticuloendothelial system)

L52 ANSWER 19 OF 24 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1957:47334 HCAPLUS
DOCUMENT NUMBER: 51:47334
ORIGINAL REFERENCE NO.: 51:88191,8820a-h
TITLE: 3,16 α -Steroid diols
INVENTOR(S): Huffman, Max N.
PATENT ASSIGNEE(S): Nepera Chemical Co., Inc.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2779773		19570129	US 1956-586637	1956 0523

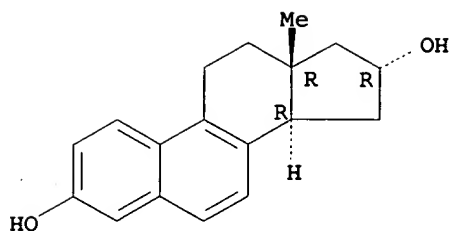
OTHER SOURCE(S): CASREACT 51:47334

AB Estrogen and androgen steroids diols with 16 α -configuration and the corresponding ether and ester derivs. have considerable physiol. activity in comparison with their β -isomers. 1,3,5(10)-Estratriene-3,16 β -diol (1 g.) in 28 ml. dry pyridine at 0° treated with 4.4 g. p-MeC₆H₄SO₂Cl, the mixture kept 2 days at room temperature, diluted with ice H₂O containing 10% NaCl, the mixture kept 24 hrs. at 5°, extracted with Et₂O, and the washed and dried extract evaporated on a steam bath gave 1.9 g. crude ditosylate, which treated with 4.8 g. freshly fused NaOEt and 92 ml. AcOH, the mixture refluxed 1 hr. at 138-50°, cooled to 5°, treated 24 hrs. with ice H₂O containing 10% NaCl, filtered, the dried residue saponified by refluxing 1 hr. with 200 ml. MeOH and 60 ml. 2.5N KOH, the MeOH evaporated, 100 ml. H₂O added, the clear solution treated with 10 ml. concentrated HCl and the pH adjusted to 5-6

with AcOH, filtered, and the dried product (0.88 g.) recrystd. from C₆H₁₄ and aqueous MeOH gave crude 3,16 α -estradiol (I), m. 213-15°, purified through the diacetate, m. 116-17°, to pure I, m. 224.0-4.5°, [α]_D²⁵ 85° (c 0.76%, 95% alc.). Similarly were prepared 1,3,5(10),6,8-estrapentaene-3,16 α -diol (II) and 1,3,5(10),7-estratetraene-3,16 α -diol (III). Alkylation of II and III gave the corresponding diacetates and dipropionates. I (46 mg.) in 30 ml. 0.5N NaOH stirred with 0.5 ml. BzCl, the mixture kept overnight at room temperature, filtered, the washed residue dried in vacuo and recrystd. from Me₂CO-C₆H₁₄ and aqueous MeOH gave 3-benzoxo-1,3,5(10)-estratrien-16 α -ol, m. 179.5-181.0°. I (150 mg.) in 6.0 ml. dry pyridine stirred 24 hrs. with 1.5 ml. BzCl, the mixture poured into ice H₂O, the oily product crystallized from alc. Me₂CO containing a trace of pyridine, and repeatedly recrystd. from Me₂CO-C₆H₁₄ and 95% alc. yielded 132 mg. 1,3,5(10)-estratriene-3,16 α -diol dibenzoate, m. 130.5-1.5°. The dipropionate, dibutyrate, divalerate, dipalmitate, distearate, bis(phenylacetate), dinaphthoate, bis(cyclopentylpropionate), and ditoluate were similarly prepared. Treatment of 118 mg. 3-methoxy-1,3,5(10)-estratrien-16 α -ol in 2 ml. pyridine with 0.2 g. p-MeC₆H₄SO₃Cl gave the corresponding 16-p-toluenesulfonate, converted by heating 1 hr. with 200 mg. fused NaOAc and 4.0 ml. AcOH to 3,16 α -estradiol 3-Me ether; 16 α -acetate, m. 123.0-3.5°. 3 β -Androstanol-16-one benzoate (575 mg.) in 300 ml. MeOH was stirred 1 hr. at room temperature with 0.39 g. NaBH₄, the mixture treated slowly with 4 ml. 50% AcOH, concentrated to 100 ml. at 100°, cooled with 100 ml. ice water and the product crystallized by standing 2 days at 0° to give 550 mg. 3 β ,16 β -androstanediol 3-benzoate (IV), m. 168-9°. IV (400 mg.) in 8 ml. dry pyridine treated with 0.8 g. p-MeC₆H₄SO₂Cl, the mixture poured into ice water, filtered, the residue dried in vacuo, refluxed 1 hr. with 1 g. fused NaOAc and 20 ml. AcOH at 137-53°, the cooled mixture extracted with Et₂O, the washed and dried extract evaporated, the residue saponified 24 hrs. in 7.5 g. KOH, 12.5 ml. H₂O, and 100 ml. MeOH, the free diol extracted with Et₂O, the washed and dried extract evaporated, and the residue purified by repeated recrystn. from Me₂CO-C₆H₁₄, MeCOEt-C₇H₁₆ and Me₂CO-C₆H₄ yielded 3 β ,16 α -androstanediol (V), m. 187.5-8.0°, [α]_D²⁵ -4° (c 0.777, 95% alc.); diacetate, m. 174.0-4.5°, [α]_D²³ -26° (c 0.963, CHCl₃). Similarly 5-androsten-3 β -ol-one benzoate or etiocholan-3 α -ol-16-one benzoate can be transformed to the corresponding 16 β -diol and epimerized to the 16 α -diol. I (38 mg.) in 8 ml. 90% MeOH and 0.8 g. K₂CO₃ refluxed, the mixture treated with 0.3 ml. Me₂SO₄, refluxed after the reaction with addnl. 0.3 ml. Me₂SO₄, the mixture distilled with 4 ml. H₂O, the turbid mixture filtered, the product washed with H₂O and dried in vacuo, taken up in Me₂CO and the solution evaporated gave 3,16 α -estradiol 3-Me ether. Other 3-ethers are similarly prepared and ether groups may be formed at the 16-HO group by use of twice the amount of dialkyl sulfates.

IT 109932-04-9, Estra-1,3,5(10),6,8-pentaene-3,16 α -diol
(esters)
RN 109932-04-9 HCAPLUS
CN Estra-1,3,5(10),6,8-pentaene-3,16-diol, (16 α)- (9CI) (CA
INDEX NAME)

Absolute stereochemistry.



(prepn. of
 CC 10 (Organic Chemistry)
 IT 1090-04-6, Estra-1,3,5(10)-triene-3,16 α -diol 109396-95-4,
 Estra-1,3,5(10),7-tetraene-3,16 α -diol 109932-04-9,
 Estra-1,3,5(10),6,8-pentaene-3,16 α -diol
 (esters)
 IT 22630-49-5, 5 α -Androstane-3 β ,16 α -diol
 54657-07-7, 5 α -Androstane-3 β ,16 α -diol, diacetate
 74111-56-1, Estra-1,3,5(10)-trien-16 α -ol, 3-methoxy-
 76820-87-6, Estra-1,3,5(10)-trien-16 α -ol, 3-methoxy-,
 acetate 109396-95-4, Estra-1,3,5(10),7-tetraene-3,16 α -diol
 109932-04-9, Estra-1,3,5(10),6,8-pentaene-3,16 α -diol
 115484-92-9, 5 α -Androstane-3 β ,16 β -diol, 3-benzoate
 (preparation of)

L52 ANSWER 20 OF 24 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1956:48821 HCAPLUS

DOCUMENT NUMBER: 50:48821

ORIGINAL REFERENCE NO.: 50:9438h-i,9439a-c

TITLE: 16-Substituted steroids. XIV. A new synthetic route to Δ 16-steroids

AUTHOR(S): Huffman, Max N.; Lott, Mary Harriet; Tillotson, Albert

CORPORATE SOURCE: Oklahoma Med. Research Foundation, Oklahoma City

SOURCE: Journal of Biological Chemistry (1955), 217, 103-6

CODEN: JBCHA3; ISSN: 0021-9258

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

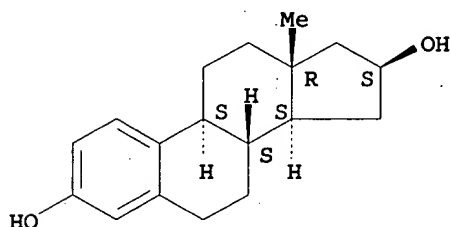
OTHER SOURCE(S): CASREACT 50:48821

AB cf. C.A. 50, 4178c. A new preparative method for ring D-substituted Δ 16-steroids is described; it involves collidine cleavage of the 16-p-toluenesulfonate to effect a double bond at C-16-C-17. This synthetic route may have wide usefulness in the steroid field. 1,3,5(10)-Estratriene-3,16 β -diol (1.00 g.) in 500 cc. 0.7N KOH at 15° shaken 10 min. with 8 cc. BzCl, the mixture held overnight at room temperature, filtered, the benzoate refluxed in 150 cc. EtOH containing 0.1 cc. pyridine and 0.1 cc. AcOH, diluted with 25 cc. water, filtered, and the filtrate concentrated to crystallization and held 24 hrs. at 5° yielded 1.23 g. 3-benzoxo-1,3,5(10)-estratrien-16 β -ol (I), m. 144-5°. I in 30 cc. dry pyridine at 0-5° treated with 3 g. solid p-MeC₆H₄SO₂Cl (II), and the mixture held 1 hr. in the ice bath, then 1 day at room temperature, diluted with 600 cc. ice water, held 1 day at 5°, and filtered yielded 1.53 g. crude tosylate (III). III (1.53 g.) refluxed 4 hrs. with 120 cc. collidine, the cooled mixture shaken with 0.7N H₂SO₄ and Et₂O, and the Et₂O phase washed yielded 900 mg. 1,3,5(10), 16-estratetraen-3-ol benzoate (IV), m. 164-7°. IV refluxed 2 hrs. with 400 cc. EtOH containing 16 cc. 2.5N KOH, diluted with 200 cc. water, the alc. removed, the residue partitioned between 600 cc. 1.1% NaHCO₃ and 800 cc. C₆H₆, the C₆H₆ phase evaporated, and the residue rebenzoylated yielded 570 mg. pure 1,3,5(10),16-estratetraen-3-ol benzoate (V), m. 177-8°.

[α]D₂₂ 84° (c 0.96, CHCl₃). V (390 mg.) refluxed 2 hrs. with 250 cc. MeOH containing 25 cc. N KOH, the mixture diluted with 75 cc. water, the MeOH removed, and the cooled residue neutralized with 1.75 cc. AcOH, held 1 day at 5°, and filtered yielded 120 mg. 1,3,5(10),16-estratetraen-3-ol, m. 130-1.5°, [α]D₂₅ 115° (c 1.50, CHCl₃); concentration of the filtrate yielded an addnl. 70 mg. m. 128.5-30°.

IT 1225-58-7, 1,3,5(10)-Estratriene-3,16 β -diol
(esters)
RN 1225-58-7 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, (16 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



CC 10 (Organic Chemistry)
IT 1225-58-7, 1,3,5(10)-Estratriene-3,16 β -diol
(esters)

L52 ANSWER 21 OF 24 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1956:36437 HCAPLUS

DOCUMENT NUMBER: 50:36437

ORIGINAL REFERENCE NO.: 50:7183a-d

TITLE: Specificity, kinetics, and inhibition of α - and α -hydroxysteroid dehydrogenases

AUTHOR(S): Talalay, Paul; Marcus, Philip I.

CORPORATE SOURCE: Univ. of Chicago

SOURCE: Journal of Biological Chemistry (1956), 218, 675-91

CODEN: JBCHA3; ISSN: 0021-9258

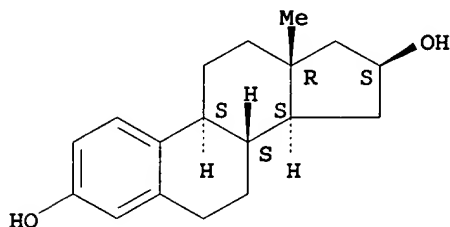
DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB cf. preceding abstract β -Hydroxysteroid dehydrogenase catalyzes the reversible DPN-linked oxidation of 3 β -, 16 β - and 17 β -hydroxy steroids. α -Hydroxysteroid dehydrogenase catalyzes the reversible DPN-linked oxidation of 3 α -hydroxysteroids of the C19, C21, and C24 series. The rates of oxidation of various steroids by these enzymes were determined. The pH of the medium affects the equilibrium point and initial velocities of the reactions catalyzed by α - and β -enzymes. The equilibrium constant for the conversion of testosterone to 4-androstene-3,17-dione is 2.6×10^{-8} and that for the conversion of androsterone to androstane-3,17-dione is 5.8×10^{-9} . The enzymes can be used for the specific enzymic microassay of selected groupings on the steroid nucleus either singly or in combination. Examples of the determination of 3 α -hydroxyl groups and 3 β - and 17 β -hydroxyl groups are given and the use of these enzymes for enzymic identification is illustrated. Michaelis consts. of α - and β -enzymes for DPN with various substrates were determined. β -Enzyme is strongly inhibited by 3,17 β -estradiol and certain related 1,3,5-estratrienes, as well as by diethylstilbestrol and diethylhexestrol. The structural requirements for β -enzyme inhibitions are present.

IT 1225-58-7, 1,3,5(10)-Estratriene-3,16 β -diol
 (β-hydroxy steroid dehydrogenase inhibition by)
 RN 1225-58-7 HCAPLUS
 CN Estra-1,3,5(10)-triene-3,16-diol, (16 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



CC 11A (Biological Chemistry: General)
 IT 50-27-1, Estriol 53-63-4, 1,3,5(10)-Estratrien-3-ol 547-81-9,
 1,3,5(10)-Estratriene-3,16 β ,17 β -triol 566-75-6,
 1,3,5(10)-Estratrien-16-one, 3,17 β -dihydroxy- 1090-04-6,
 1,3,5(10)-Estratriene-3,16 α -diol 1225-58-7,
 1,3,5(10)-Estratriene-3,16 β -diol 2529-64-8,
 1,3,5(10)-Estratrien-17 β -ol 5635-50-7, Phenol,
 4,4'-(1,2-diethylethylene)di- 6898-97-1, 4,4'-Stilbenediol,
 α,α' -diethyl- 20576-40-3, 1,3,5(10)-Estratrien-
 17 α -ol
 (β-hydroxy steroid dehydrogenase inhibition by)

L52 ANSWER 22 OF 24 HCAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 1956:28422 HCAPLUS
 DOCUMENT NUMBER: 50:28422
 ORIGINAL REFERENCE NO.: 50:5784i,5785a-d
 TITLE: Estrogenic compounds
 INVENTOR(S): Huffman, Max N.
 PATENT ASSIGNEE(S): Nepera Chemical Co., Inc.
 DOCUMENT TYPE: Patent
 LANGUAGE: Unavailable
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

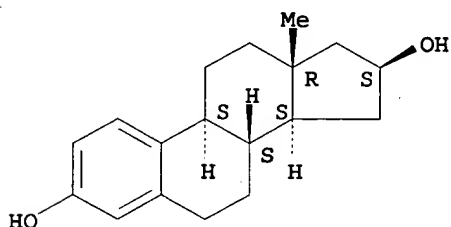
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2705239		19550329	US 1953-354409	1953 0511

AB 16-Estrone (I) (250 mg.) hydrogenated with PtO₂ in 0.5N NaOH during 12 hrs. at 25°, then left 24 hrs. at 25°, the mixture acidified, extracted with Et₂O, the crystalline residue refluxed 3 hrs. with 0.24 g. HO₂CCH₂ONH₂.0.5HCl, 0.37 g. KOAc, and 40 cc. aqueous PrOH (1:3), left 24 hrs. at 25°, extracted with Et₂O, the extract treated with 3% NaHCO₃ to remove unchanged material, washed, and the product crystallized yielded 3,16-estradiol (II), m. 224-6° (from Me₂CO). A mixture of estrone and I (800 mg.) reduced 30 min. in MeOH with 0.2 g. NaBH₄, stirred 0.5 hr., 15 cc. N NaOH added, and the mixture left at room temperature 24 hrs. gave, after a lengthy purification, 154 mg. II. II with NaOH and BzCl in H₂O gave the 3-benzoate (III), needles, m. 145-6°, saponified to II. Extremely pure II m. 227-7.5°, [α]_D²¹ 79° (95% EtOH). Other 3-aryl esters of II may be prepared by this method whereas the 3-aliphatic esters may be prepared by catalytic reduction of the corresponding ester of I. II (38 mg.) covered with 8 cc. 90% MeOH and 0.8 g. K₂CO₃, and refluxed 45 min. with

addition of Me₂SO₄ yielded the 3-Me ether of II as an oil (IV), giving with Ac₂O in C₅H₅N 17 mg. 3-methoxy-16 β -acetoxy-1,3,5-estratriene (V), m. 130-1°. To prepare 16-esters of II, a compound such as the 3-benzyl ether of II was treated with an acid chloride or anhydride and the benzyl group removed by hydrogenolysis with Pd-C. The diesters of II were prepared by using a large excess of the corresponding acid anhydride in C₅H₅N. The 3-Me ether of I (190 mg.) with NaBH₄ in MeOH gave IV, m. 103.5-4.0°. IV with Ac₂O-C₅H₅N yielded V, m. 132-2.5°, saponified to IV. I gave the 3-benzyl ether, reduced with NaBH₄ to the 3-benzyl ether of II, m. 148-9°.

IT 1225-58-7, 1,3,5(10)-Estratriene-3,16 β -diol
(preparation of)
RN 1225-58-7 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, (16 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



CC 10 (Organic Chemistry)
IT 1225-58-7, 1,3,5(10)-Estratriene-3,16 β -diol
1225-58-7, 3,16 β -Estradiol 1229-33-0,
1,3,5(10)-Estratrien-16 β -ol, 3-methoxy-
(preparation of)

L52 ANSWER 23 OF 24 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1956:8696 HCAPLUS

DOCUMENT NUMBER: 50:8696

ORIGINAL REFERENCE NO.: 50:1874e-f

TITLE: Application of the Favorskii reaction to steroid 3-ketones

AUTHOR(S): Evans, D. E.; de Paulet, A. C.; Shoppee, C. W.; Winternitz, F.

CORPORATE SOURCE: Univ. Wales

SOURCE: Chemistry & Industry (London, United Kingdom) (1955) 355-6

CODEN: CHINAG; ISSN: 0009-3068

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

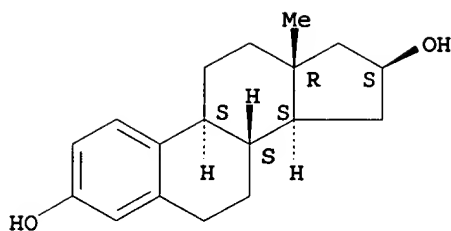
AB cf. Bulletin society chim. France 1954, 288. 4 β -Bromocoprostan-3-one with NaOMe yields Me A-norcoprostan-3-carboxylate (I), m. 67-8°, and the isomeric 2-carboxylate (II), a liquid Barbier-Wieland degradation of I yields A-norcoprostan-3-one, m. 73°. A similar degradation of II should furnish A-norcoprostan-2-one.

IT 1225-58-7, 1,3,5(10)-Estratriene-3,16 β -diol
(and esters)

RN 1225-58-7 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, (16 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



CC 10 (Organic Chemistry)
 IT 1225-58-7, 1,3,5(10)-Estratriene-3,16 β -diol
 (and esters)

L52 ANSWER 24 OF 24 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1955:85867 HCAPLUS

DOCUMENT NUMBER: 49:85867

ORIGINAL REFERENCE NO.: 49:16212b-f

TITLE: Depression of estrone-induced uterine growth by phenolic estrogens with oxygenated functions at positions 6 or 16: the impeded estrogens

AUTHOR(S): Huggins, Charles; Jensen, Elwood V.

CORPORATE SOURCE: Univ. of Chicago

SOURCE: Journal of Experimental Medicine (1955), 102, 335-46

CODEN: JEMEAV; ISSN: 0022-1007

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

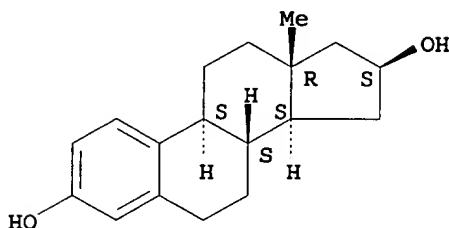
AB Thirty-eight-day-old, hypophysectomized rats, maintained on a ration free of growth-promoting steroids, were injected subcutaneously for 7 days with estrogenic substances (I). At necropsy, the spleen, preputial glands, vagina, and the uterus were excised and weighed, the N content of the uterus was determined, and the vaginal epithelium was examined microscopically. The growth of the uterus was related to the dosage of I which differed in the number of substituent groups and in their state of oxidation. A small increase of I dosage above the threshold amount resulted in a sharp increase of uterine growth succeeded by a gentle terrace-like rise until maximum growth was attained. The following I, termed unimpeded I, together with their terrace-point dosage, stimulated growth of the uterus: 17 β -estradiol, 0.025 γ ; estrone, 0.25; equilin, 0.25; 6-dehydroestrone, 2.5; D-equilenin, 5; 4-hydroxyestradiol-17 β , 10; 7-ketoestrone, 10; 17 α -estradiol, 10; 17-deoxyestradiol, 10; 16-estrone, 10; Δ -16,17-deoxyestradiol, 20; 16-ketoestradiol-17 β , 25; 3-deoxyestradiol-17 β , 25; 3-deoxyestrone, 50; 3-deoxyestradiol-17 α , 100; 16-ketoestrone, >100. The presence of 2 H atoms at C6 was required for full physiol. activity of I. In contrast a I series having either a C:O group at position 6 or a C-OH at 16, when injected simultaneously with estrone, caused a moderate depression of uterine growth below that induced by estrone alone. These impeded compds. were: 6-ketoestradiol-17 β , 6-ketoestrone, estriol, 16-epiestriol, 17-epiestriol, 16 α -estradiol, 16 β -estradiol. The optimum dosage of the compds. in the above order were 1.0 γ , 5.0, 2.5, 2.5, 2.5, 5.0, and 5.0 γ , resp. The depression of uterine growth manifested itself both in a decrease in weight and in total N content. The maximum inhibition of uterine growth was 26-43%. These impeded I did not depress the growth of or the amount of cornification of the epithelial cells in the vagina. The impeded I were 3-hydroxyestratriene derivs. possessing either a C:O group at position 6 or a C-OH group at position 16.

IT 1225-58-7, 1,3,5(10)-Estratriene-3,16 β -diol

(effect on uterus)

RN 1225-58-7 HCAPLUS
 CN Estradiol, 1,3,5(10)-triene-3,16-diol, (16 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



CC 11H (Biological Chemistry: Pharmacology)
 IT 50-27-1, Estriol 53-45-2, 1,3,5(10)-Estratrien-17-one 53-63-4, Estradiol, 17-deoxy- 53-63-4, 1,3,5(10)-Estratrien-3-ol 57-91-0, 17 α -Estradiol 474-86-2, Equilin 517-09-9, Equilenin 547-81-9, 1,3,5(10)-Estratriene-3,16 β ,17 β -triol 566-75-6, 1,3,5(10)-Estratrien-16-one, 3,17 β -dihydroxy- 571-92-6, 1,3,5(10)-Estratrien-6-one, 3,17 β -dihydroxy- 1090-04-6, 1,3,5(10)-Estratriene-3,16 α -diol 1150-90-9, 1,3,5(10),16-Estratetraen-3-ol 1150-90-9, Δ 16-Estradiol, 17-deoxy- 1225-58-7, 1,3,5(10)-Estratriene-3,16 β -diol 1228-72-4, 1,3,5(10)-Estratriene-3,16 α ,17 α -triol 1228-73-5, 1,3,5(10)-Estratriene-16,17-dione, 3-hydroxy- 1476-34-2, 1,3,5(10)-Estratriene-6,17-dione, 3-hydroxy- 2208-12-0, 1,3,5(10),6-Estratetraen-17-one, 3-hydroxy- 2464-15-5, 1,3,5(10)-Estratriene-7,17-dione, 3-hydroxy- 2529-64-8, 1,3,5(10)-Estratrien-17 β -ol 2529-64-8, Estradiol, 3-deoxy- 3601-97-6, 1,3,5(10)-Estratrien-16-one, 3-hydroxy- 5976-61-4, 1,3,5(10)-Estratrien-3,4,17 β -triol 5976-61-4, Estradiol, 4-hydroxy- 20576-40-3, 1,3,5(10)-Estratrien-17 α -ol 20576-40-3, 17 α -Estradiol, 3-deoxy- (effect on uterus)

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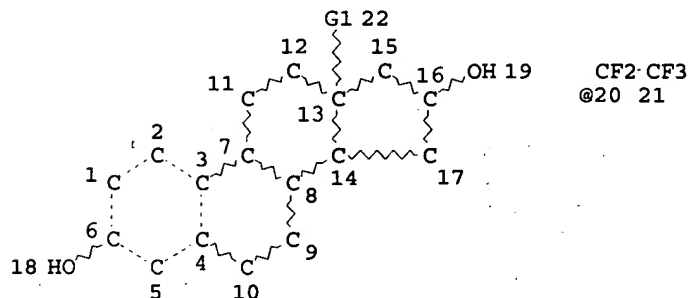
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L13

L14

SCR 1844

STR



VAR G1=ME/ET/CF3/20

NODE ATTRIBUTES:

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DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 22

STEREO ATTRIBUTES: NONE

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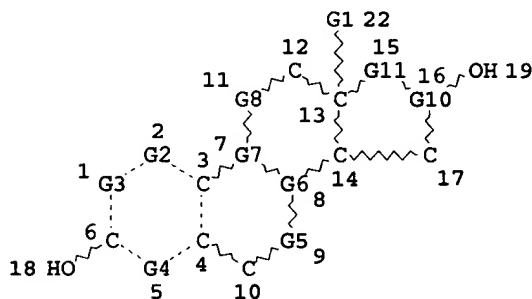
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C~OEt C~Ak C~O~Ak C~CF2 CF3 C~Ak~F
 @33 34 @35 36 @37 38 39 @42 41 40 @43 44 45

C~Cy C~CN C~Et C~O~NO2 C~CH2Cl
 @46 47 @48 49 @50 51 @52 53 54 @55 56 57

C~G9 C~S~Ak S @62
 @58 59 @60 61 63



C~CH2 CN C~F
 @64 65 66 @67 68

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 VAR G3=CH/23/27/35/37
 VAR G4=CH/23/35/25/42/37
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GRAPH ATTRIBUTES:
 RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 68

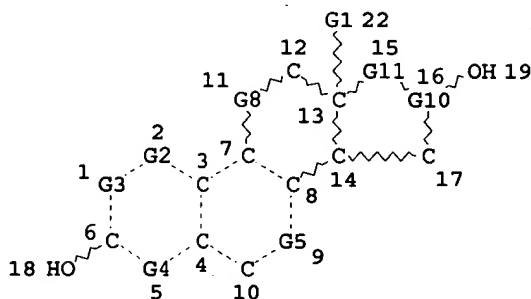
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C~Cy C~CN C~Et C~O~NO2 C~CH2Cl
 @46 47 48 49 50 51 @52 53 54 @55 56 57

C~G9 C~S~Ak S @62
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C~CH2·CN C~F
 @64 65 66 @67 68

VAR G1=ME/ET/CF3/20
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NODE ATTRIBUTES:

CONNECT IS E2 RC AT 61
 CONNECT IS E1 RC AT 62
 DEFAULT MLEVEL IS ATOM
 GGCAT IS UNS AT 47
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 68

STEREO ATTRIBUTES: NONE

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 L33 24 SEA FILE=HCAPLUS ABB=ON PLU=ON L16
 L34 46181 SEA FILE=HCAPLUS ABB=ON PLU=ON STEROID?/SC,SX
 L35 362 SEA FILE=HCAPLUS ABB=ON PLU=ON L31 AND L34
 L36 316 SEA FILE=HCAPLUS ABB=ON PLU=ON L32 AND L34
 L37 2051502 SEA FILE=HCAPLUS ABB=ON PLU=ON PHARMA?/SC,SX
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L53 ANSWER 1 OF 16 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2005:1260644 HCAPLUS
DOCUMENT NUMBER: 144:23044
TITLE: Preparation of aminosulfonyl- or
aminosulfonylamino-substituted phenyl esters
as estriol and estetrol prodrugs
INVENTOR(S): Wyrwa, Ralf; Droescher, Peter; Ring, Sven;
Elger, Walter; Schneider, Birgitt; Hillisch,
Alexander; Reddersen, Gudrun
PATENT ASSIGNEE(S): Schering Aktiengesellschaft, Germany
SOURCE: PCT Int. Appl., 43 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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WO 2005113576	A1	20051201	WO 2005-EP5258	2005 0510
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RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
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PRIORITY APPLN. INFO.:			DE 2004-102004025985A	2004 0521
			US 2004-572972P	P 2004 0521

OTHER SOURCE(S): CASREACT 144:23044
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT

AB The invention relates to estriol and estetrol prodrugs I [A = (CH₂)_n; n = 0 - 4; when R₁ = SO₂NH₂, NHSO₂NH₂, then R₂, R₃, X, X₁ = H, halogen, CN, NO₂, C₁-5-alkyl, CpF_{2p+1}, OC(:O)R₂₀, CO₂R₂₀, OR₂₀, C(:O)NHR₂₀, OC(:O)NHR₂₁; when R₂ = SO₂NH₂, NHSO₂NH₂, then R₁, R₃, X, X₁ = H, halogen, CN, NO₂, C₁-5-alkyl, CpF_{2p+1}, OC(:O)R₂₀, CO₂R₂₀, OR₂₀, C(:O)NHR₂₀, OC(:O)NHR₂₁; when R₃ = SO₂NH₂, NHSO₂NH₂, then R₁, R₂, X, X₁ = H, halogen, CN, NO₂, C₁-5-alkyl, CpF_{2p+1}, OC(:O)R₂₀, CO₂R₂₀, OR₂₀, C(:O)NHR₂₀, OC(:O)NHR₂₁; p = 1 - 3; R₁₅ = H, OH, tri(C₁-6-alkyl)silyloxy, OC(:O)R₂₀, C₂-5-heterocyclkoalkoxy; R₁₆, R₁₇ = OH, tri(C₁-6-alkyl)silyloxy, OC(:O)R₂₀, C₂-5-heterocyclkoalkoxy; R₂₀ = H; R₂₀, R₂₁, R₂₂ = C₁-5-alkyl, C₃-8-cycloalkyl, aryl, (C₁-4-alkylene)aryl, (C₁-4-alkylene)-(C₃-8-cycloalkyl), (C₃-8-cycloalkylene)-(C₁-4-alkyl)], II [R₄ = OH, tri(C₁-6-alkyl)silyloxy, OC(:O)R₂₀, C₂-5-heterocyclkoalkoxy], III and IV, and their pharmaceutically acceptable salts, the method for production thereof, pharmaceutical compns. comprising said compds. and the use thereof for production of medicaments with **estrogenic effect**. Thus, 3,16 α -dihydroxyestra-1,3,5(10)-trien-17 β -yl 3'sulfamoylbenzoate [II; R₄ = OH, R₁₅ = H, R₁₆ = α -OH, Y = (O₂CC₆H₄SO₂NH₂-3)- β] was prepared from 3,16 α -di[(tert-butylsilyl)oxy]estra-1,3,5(10)-trien-17 β -ol via acylation with 3-(ClSO₂)C₆H₄COCl in CHCl₃ containing pyridine and amidation with aqueous NH₃. The bioactivity of II [R₄ = OH, R₁₅ = H, R₁₆ = α -OH, Y = (O₂CC₆H₄SO₂NH₂-3)- β] was determined [relative binding affinity (RBA) to erythrocytes: RBA = 0.5; IC₅₀ = 600 nM vs. carboanhydrase].

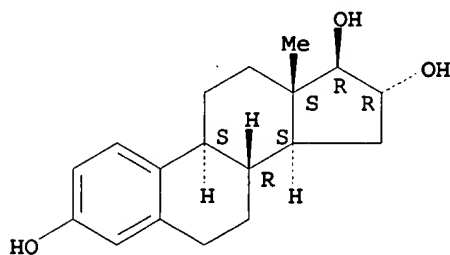
IT 50-27-1, Estriol

RL: PAC (Pharmacological activity); RCT (Reactant); THU (Therapeutic use); BIOL (Biological study); RACT (Reactant or reagent); USES (Uses)
(acylation of, by (aminosulfonylphenyl)- or (aminosulfonylaminophenyl) carboxylic acids; preparation of aminosulfonyl- or aminosulfonylamino-substituted Ph esters as estriol and estetrol prodrugs)

RN 50-27-1 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16,17-triol, (16 α ,17 β)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.



IT 15183-37-6DP, Estetrol, prodrugs 870127-75-6P

870127-76-7P 870127-83-6P 870127-85-8P

870127-86-9P 870127-89-2P 870127-90-5P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation);

THU (Therapeutic use); BIOL (Biological study); PREP

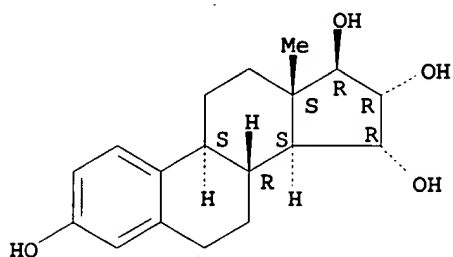
(Preparation); USES (Uses)

(preparation of aminosulfonyl- or aminosulfonylamino-substituted Ph esters as estriol and estetrol prodrugs)

RN 15183-37-6 HCAPLUS

CN Estr-1,3,5(10)-triene-3,15,16,17-tetrol,
(15 α ,16 α ,17 β)- (9CI) (CA INDEX NAME)

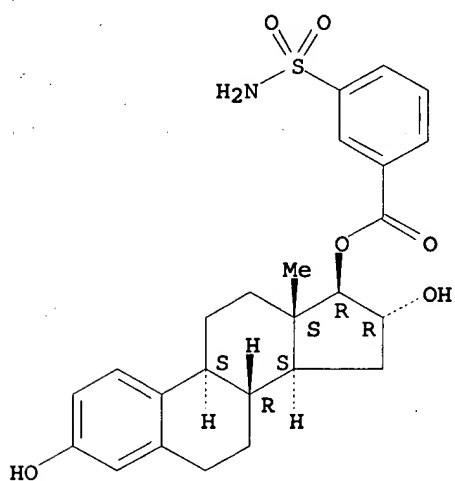
Absolute stereochemistry.



RN 870127-75-6 HCAPLUS

CN Estr-1,3,5(10)-triene-3,16,17-triol, 17-[3-(aminosulfonyl)benzoate], (16 α ,17 β)- (9CI) (CA INDEX NAME)

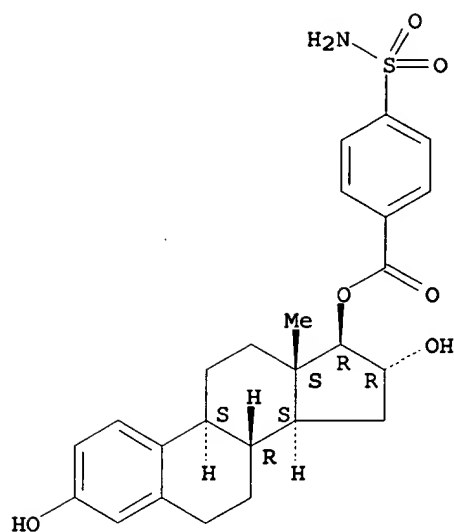
Absolute stereochemistry.



RN 870127-76-7 HCAPLUS

CN Estr-1,3,5(10)-triene-3,16,17-triol, 17-[4-(aminosulfonyl)benzoate], (16 α ,17 β)- (9CI) (CA INDEX NAME)

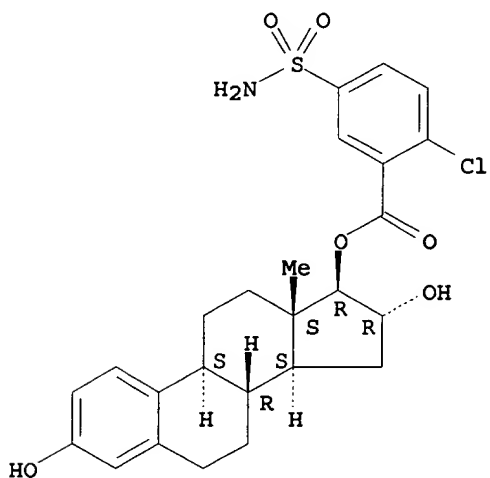
Absolute stereochemistry.



RN 870127-83-6 HCAPLUS

CN Estrone-1,3,5(10)-triene-3,16,17-triol, 17-[5-(aminosulfonyl)-2-chlorobenzoate], (16 α ,17 β)- (9CI) (CA INDEX NAME)

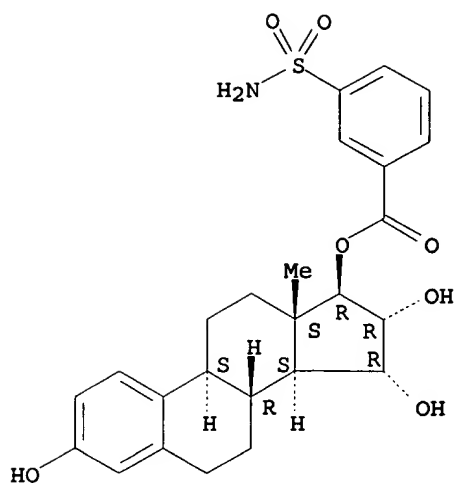
Absolute stereochemistry.



RN 870127-85-8 HCAPLUS

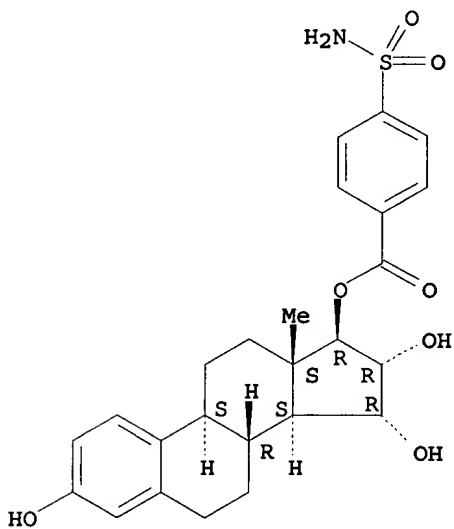
CN Estrone-1,3,5(10)-triene-3,15,16,17-tetrol, 17-[3-(aminosulfonyl)benzoate], (15 α ,16 α ,17 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



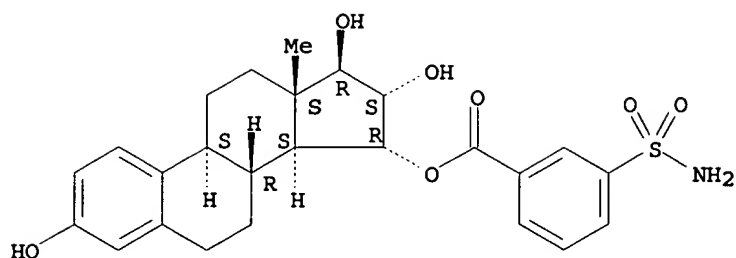
RN 870127-86-9 HCAPLUS
 CN Estrone-1,3,5(10)-triene-3,15,16,17-tetrol, 17-[4-(aminosulfonyl)benzoate], (15 α ,16 α ,17 β)- (9CI)
 (CA INDEX NAME)

Absolute stereochemistry.



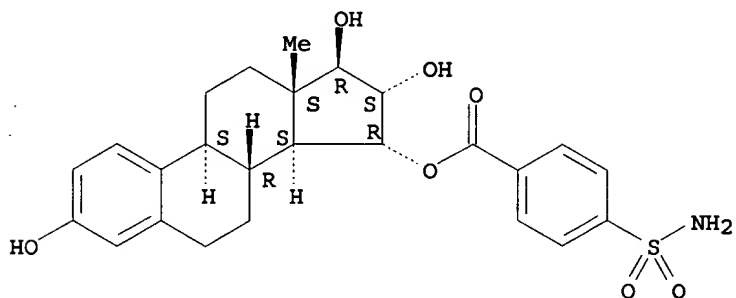
RN 870127-89-2 HCAPLUS
 CN Estrone-1,3,5(10)-triene-3,15,16,17-tetrol, 15-[3-(aminosulfonyl)benzoate], (15 α ,16 α ,17 β)- (9CI)
 (CA INDEX NAME)

Absolute stereochemistry.



RN 870127-90-5 HCAPLUS
 CN Estrone-1,3,5(10)-triene-3,15,16,17-tetrol, 15-[4-(aminosulfonyl)benzoate], (15 α ,16 α ,17 β)- (9CI)
 (CA INDEX NAME)

Absolute stereochemistry.



IC ICM C07J041-00
 ICS A61K031-565; A61P005-30
 CC 32-3 (Steroids)
 Section cross-reference(s): 1, 2, 25, 63
 ST prodrug estriol estetrol aminosulfonylphenyl
 aminosulfonylaminophenyl ester prepn; **estrogenic**
 aminosulfonylphenyl aminosulfonylaminophenyl ester prodrug prepn
 IT **Estrogens**
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (acylation of, by aminosulfonylphenyl and
 aminosulfonylaminophenylalkanoic acids; preparation of
 aminosulfonyl- or aminosulfonylamino-substituted Ph esters as
 estriol and estetrol prodrugs)
 IT Carboxylic acids, reactions
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (aminosulfonylphenyl and aminosulfonylaminophenyl, acylation
 by, of **estrogens**; preparation of aminosulfonyl- or
 aminosulfonylamino-substituted Ph esters as estriol and
 estetrol prodrugs)
 IT Progestogens
 RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
 (Biological study); USES (Uses)
 (combination chemotherapy of, with **estrogen** prodrugs;
 preparation of aminosulfonyl- or aminosulfonylamino-substituted Ph
 esters as estriol and estetrol prodrugs)
 IT Acylation
 (of **estrogens** by aminosulfonylaminophenyl- and
 aminosulfonylphenylalkanoic acids; preparation of aminosulfonyl- or
 aminosulfonylamino-substituted Ph esters as estriol and
 estetrol prodrugs)
 IT Combination chemotherapy
 (of gestagens with **estrogen** prodrugs; preparation of

- aminosulfonyl- or aminosulfonylamino-substituted Ph esters as estriol and estetrol prodrugs)
- IT **Estrogen receptors**
RL: BSU (Biological study, unclassified); BIOL (Biological study) (α , relative binding affinity; preparation of aminosulfonyl- or aminosulfonylamino-substituted Ph esters as estriol and estetrol prodrugs)
- IT **Estrogen receptors**
RL: BSU (Biological study, unclassified); BIOL (Biological study) (β , relative binding affinity; preparation of aminosulfonyl- or aminosulfonylamino-substituted Ph esters as estriol and estetrol prodrugs)
- IT **50-27-1, Estriol**
RL: PAC (Pharmacological activity); RCT (Reactant); THU (Therapeutic use); BIOL (Biological study); RACT (Reactant or reagent); USES (Uses)
(acylation of, by (aminosulfonylphenyl)- or (aminosulfonylamino) carboxylic acids; preparation of aminosulfonyl- or aminosulfonylamino-substituted Ph esters as estriol and estetrol prodrugs)
- IT **57-83-0, Progesterone, biological studies**
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(combination chemotherapy of, with **estrogen** prodrugs; preparation of aminosulfonyl- or aminosulfonylamino-substituted Ph esters as estriol and estetrol prodrugs)
- IT **68-22-4, Norethisterone 71-58-9, Medroxyprogesterone acetate 302-22-7, Chlormadinone acetate 427-51-0, Cyproterone acetate 797-63-7, Levonorgestrel 60282-87-3, Gestodene 65928-58-7, Dienogest 67392-87-4, Drospirenone**
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(combination chemotherapy of, with **estrogen** prodrugs; preparation of aminosulfonyl- or aminosulfonylamino-substituted Ph esters as estriol and estetrol prodrugs)
- IT **15183-37-6DP, Estetrol, prodrugs 870127-75-6P 870127-76-7P 870127-77-8P 870127-78-9P 870127-79-0P 870127-80-3P 870127-81-4P 870127-82-5P 870127-83-6P 870127-84-7P 870127-85-8P 870127-86-9P 870127-87-0P 870127-88-1P 870127-89-2P 870127-90-5P 870127-91-6P 870127-92-7P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of aminosulfonyl- or aminosulfonylamino-substituted Ph esters as estriol and estetrol prodrugs)
- REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L53 ANSWER 2 OF 16 HCAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 2005:902909 HCAPLUS
 DOCUMENT NUMBER: 143:230061
 TITLE: Preparation of 7 α -substituted 17-alkylene-16 α -hydroxysteroidal **estrogens** for cancer treatment
 INVENTOR(S): Pettersson, Lars
 PATENT ASSIGNEE(S): Innoventus Project AB, Swed.
 SOURCE: PCT Int. Appl., 80 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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WO 2005077968

A2

20050825

WO 2005-SE188

2005
0211

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ,
CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG,
ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP,
KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD,
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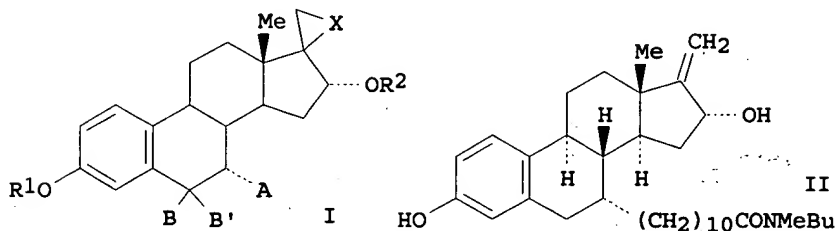
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2004
0213

OTHER SOURCE(S):

MARPAT 143:230061

GI



AB 7 α -Substituted 17-alkylene-16 α -hydroxysteroidal estrogens of formula I [A = 8-22 atom substituent; B, B' = H, OH, alkoxy, etc.; X = methylene, bond; R1 = H, metabolically unstable group; R2 = H, acyl, benzoyl] are prepared which exhibit anti-estrogenic properties. The present invention also relates to use of said compds. as a medicament, and for the treatment of estrogen dependent disorders, a pharmaceutical composition comprising one or more of said compds. and a method of treatment. Thus, II was prepared, and showed 61% antagonism in vivo in immature female mice.

IT 862700-33-2P 862700-40-1P 862700-44-5P

862700-47-8P 862700-49-0P 862700-51-4P

862700-53-6P 862700-55-8P 862700-57-0P

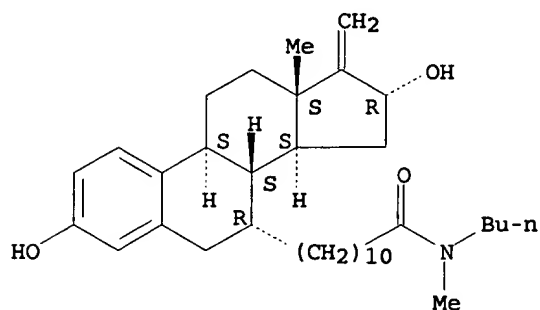
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(preparation of antiestrogenic 17-alkylene-16 α -hydroxyestratrienes for cancer treatment)

RN 862700-33-2 HCAPLUS

CN Estra-1,3,5(10)-triene-7-undecanamide, N-butyl-3,16-dihydroxy-N-methyl-17-methylene-, (7 α ,16 α)- (9CI) (CA INDEX NAME)

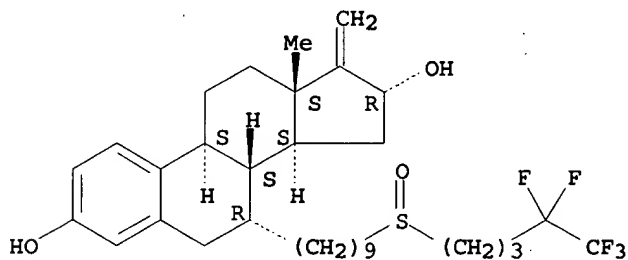
Absolute stereochemistry.



RN 862700-40-1 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 17-methylene-7-[9-[(4,4,5,5,5-pentafluoropentyl)sulfinyl]nonyl]-, (7 α ,16 α)- (9CI) (CA INDEX NAME)

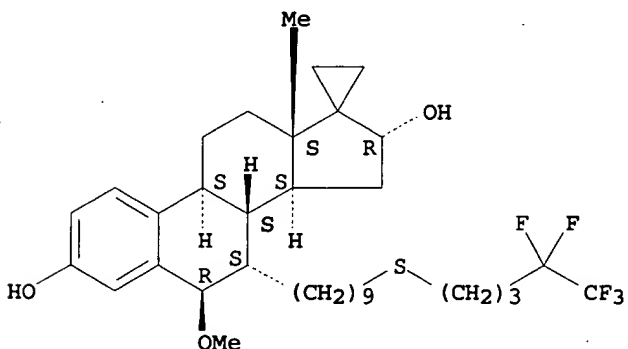
Absolute stereochemistry.



RN 862700-44-5 HCAPLUS

CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-3,16-diol, 6-methoxy-7-[9-[(4,4,5,5,5-pentafluoropentyl)thio]nonyl]-, (6 β ,7 α ,16 α)- (9CI) (CA INDEX NAME)

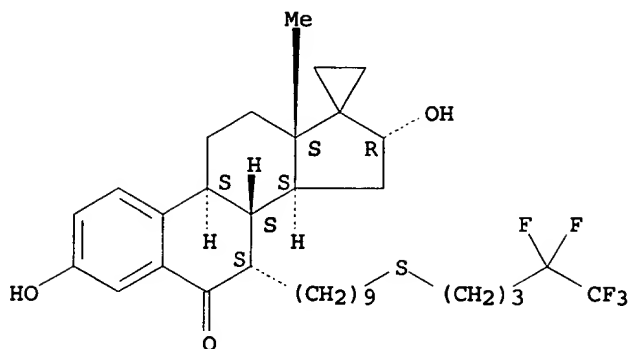
Absolute stereochemistry.



RN 862700-47-8 HCAPLUS

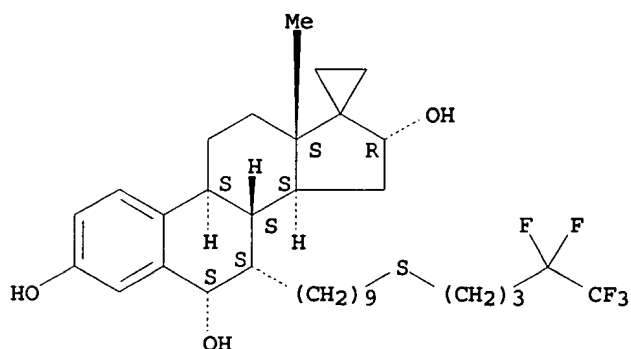
CN 17,21-Cyclo-19-norpregna-1,3,5(10)-trien-6-one, 3,16-dihydroxy-7-[9-[(4,4,5,5,5-pentafluoropentyl)thio]nonyl]-, (7 α ,16 α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



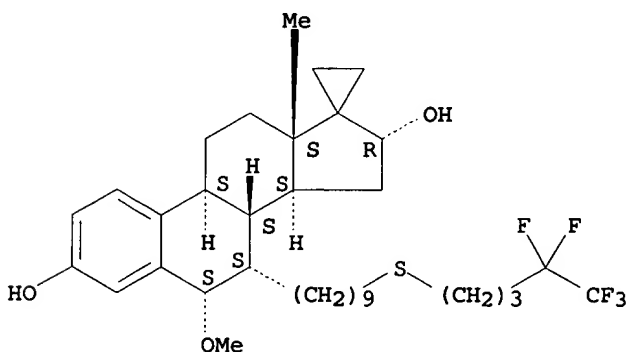
RN 862700-49-0 HCAPLUS
 CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-3,6,16-triol,
 7-[9-[(4,4,5,5,5-pentafluoropentyl)thio]nonyl]-,
 (6 α ,7 α ,16 α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 862700-51-4 HCAPLUS
 CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-3,16-diol,
 6-methoxy-7-[9-[(4,4,5,5,5-pentafluoropentyl)thio]nonyl]-,
 (6 α ,7 α ,16 α)- (9CI) (CA INDEX NAME)

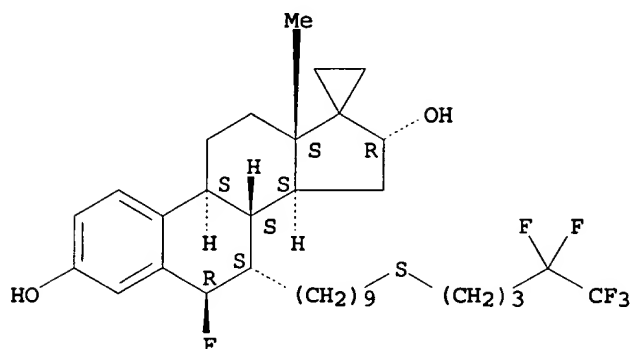
Absolute stereochemistry.



RN 862700-53-6 HCAPLUS
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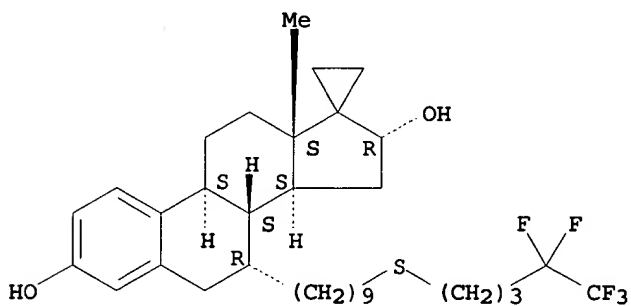
6-fluoro-7-[9-[(4,4,5,5,5-pentafluoropentyl)thio]nonyl]-,
(6 β ,7 α ,16 α)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



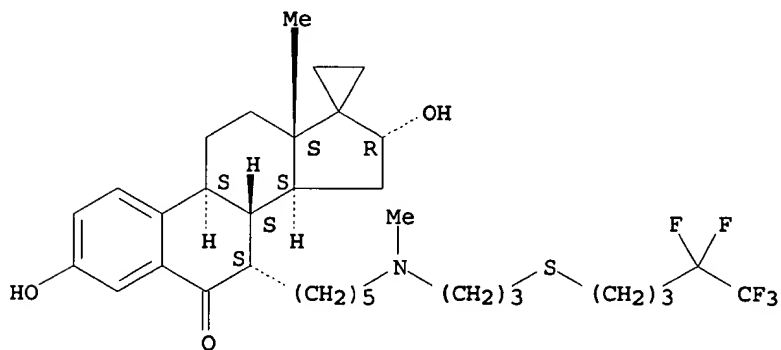
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CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-3,16-diol,
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(7 α ,16 α)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



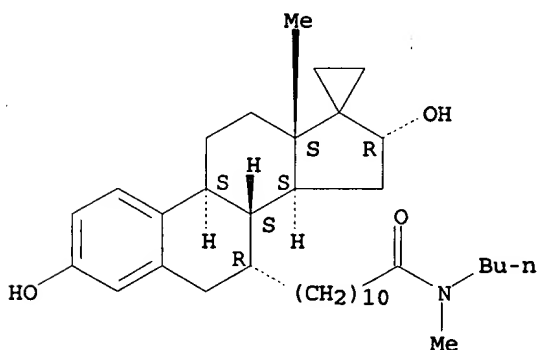
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pentafluoropentyl)thio]propyl]amino]pentyl]-, (7 α ,16 α)-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.



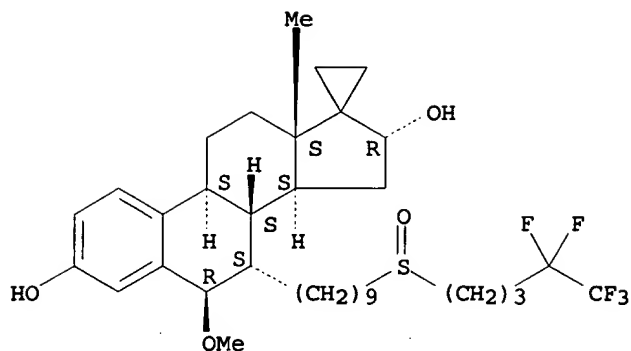
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 RL: PAC (Pharmacological activity); SPN (Synthetic preparation);
 THU (Therapeutic use); BIOL (Biological study); PREP
 (Preparation); USES (Uses)
 (preparation of antiestrogenic 17-alkylene-16 α -
 hydroxyestratrienes for cancer treatment)
 RN 862700-38-7 HCAPLUS
 CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-7-undecanamide,
 N-butyl-3,16-dihydroxy-N-methyl-, (7 α ,16 α)- (9CI) (CA
 INDEX NAME)

Absolute stereochemistry.



RN 862700-46-7 HCAPLUS
 CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-3,16-diol,
 6-methoxy-7-[9-[(4,4,5,5,5-pentafluoropentyl)sulfinyl]nonyl]-,
 (6 β ,7 α ,16 α)- (9CI) (CA INDEX NAME)

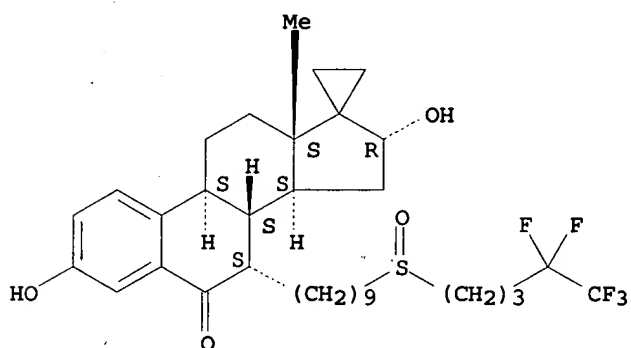
Absolute stereochemistry.



RN 862700-48-9 HCAPLUS

CN 17,21-Cyclo-19-norpregna-1,3,5(10)-trien-6-one,
3,16-dihydroxy-7-[9-[(4,4,5,5,5-pentafluoropentyl)sulfinyl]nonyl]-,
(7 α ,16 α)-(9CI) (CA INDEX NAME)

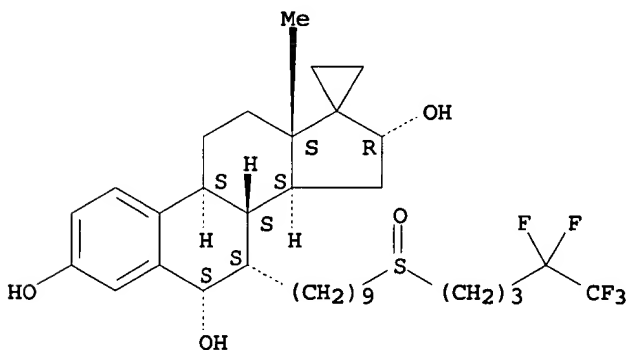
Absolute stereochemistry.



RN 862700-50-3 HCAPLUS

CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-3,6,16-triol,
7-[9-[(4,4,5,5,5-pentafluoropentyl)sulfinyl]nonyl]-,
(6 α ,7 α ,16 α)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

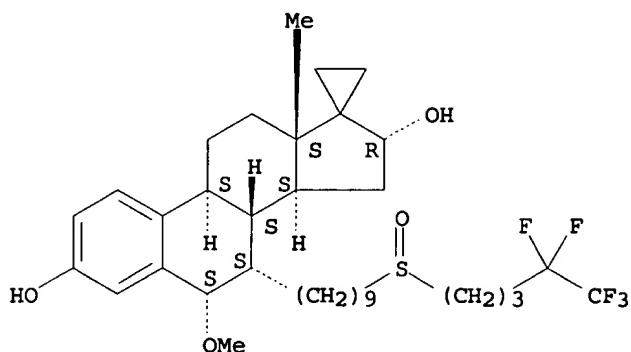


RN 862700-52-5 HCAPLUS

CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-3,16-diol,
6-methoxy-7-[9-[(4,4,5,5,5-pentafluoropentyl)sulfinyl]nonyl]-,
(6 α ,7 α ,16 α)-(9CI) (CA INDEX NAME)

(6 α ,7 α ,16 α)- (9CI) (CA INDEX NAME)

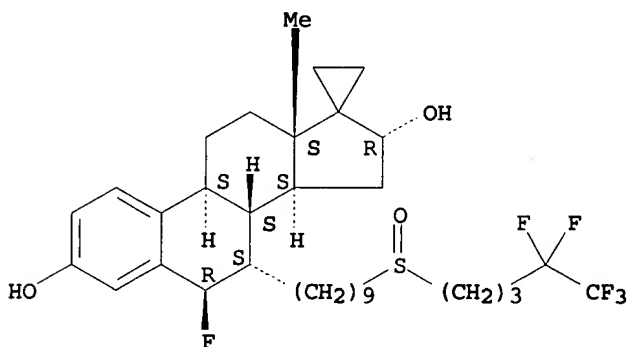
Absolute stereochemistry.



RN 862700-54-7 HCAPLUS

CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-3,16-diol,
6-fluoro-7-[9-[(4,4,5,5,5-pentafluoropentyl)sulfinyl]nonyl]-,
(6 β ,7 α ,16 α)- (9CI) (CA INDEX NAME)

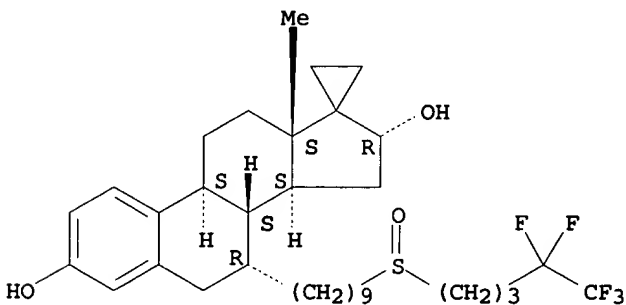
Absolute stereochemistry.



RN 862700-56-9 HCAPLUS

CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-3,16-diol,
7-[9-[(4,4,5,5,5-pentafluoropentyl)sulfinyl]nonyl]-,
(7 α ,16 α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

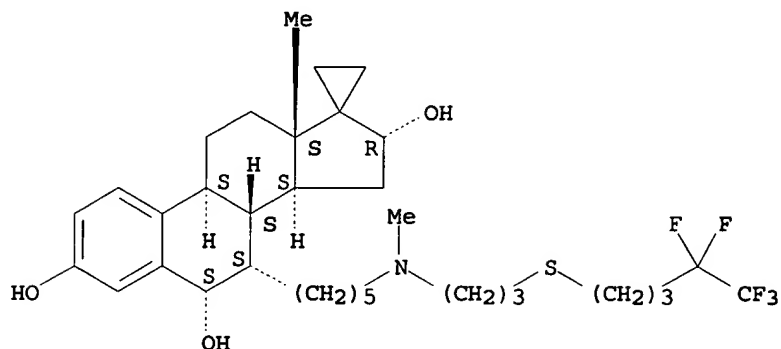


RN 862700-59-2 HCAPLUS

CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-3,6,16-triol,
7-[9-[(4,4,5,5,5-pentafluoropentyl)sulfinyl]nonyl]-

7-[5-[methyl[3-[(4,4,5,5,5-pentafluoropentyl)thio]propyl]amino]pentyl]-, (6 α ,7 α ,16 α)- (9CI) (CA INDEX NAME)

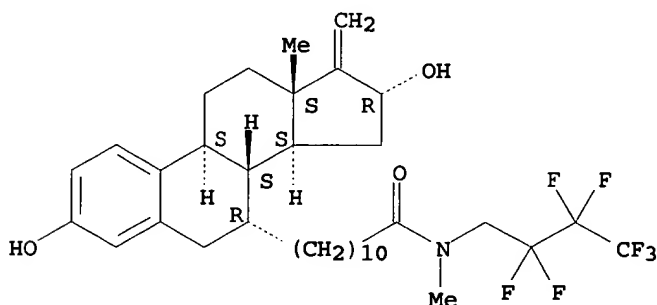
Absolute stereochemistry.



RN 862701-26-6 HCAPLUS

CN Estra-1,3,5(10)-triene-7-undecanamide, N-(2,2,3,3,4,4,4-heptafluorobutyl)-3,16-dihydroxy-N-methyl-17-methylene-, (7 α ,16 α)- (9CI) (CA INDEX NAME)

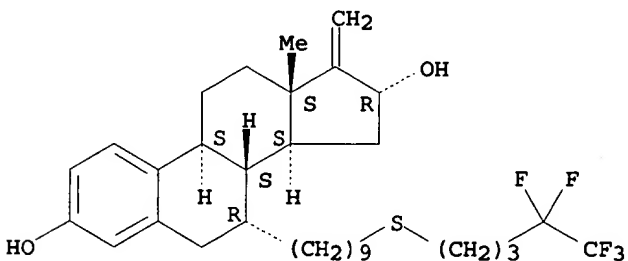
Absolute stereochemistry.



RN 862701-28-8 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 17-methylene-7-[9-[(4,4,5,5,5-pentafluoropentyl)thio]nonyl]-, (7 α ,16 α)- (9CI) (CA INDEX NAME)

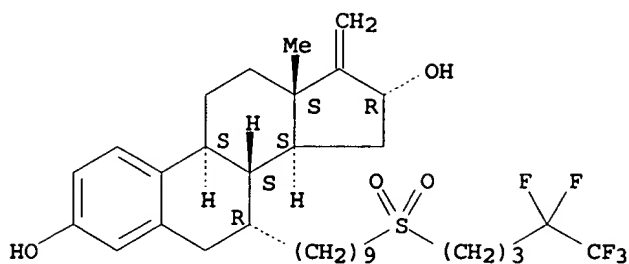
Absolute stereochemistry.



RN 862701-34-6 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 17-methylene-7-[9-[(4,4,5,5,5-pentafluoropentyl)sulfonyl]nonyl]-, (7 α ,16 α)- (9CI) (CA INDEX NAME)

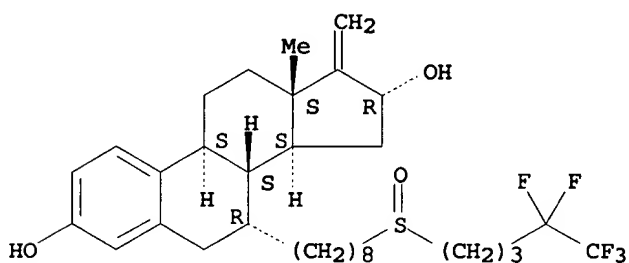
Absolute stereochemistry.



RN 862701-36-8 HCAPLUS

CN Estradiol, 17-methylene-7-[8-[(4,4,5,5,5-pentafluoropentyl)sulfinyl]octyl]-, (7 α ,16 α)- (9CI)
(CA INDEX NAME)

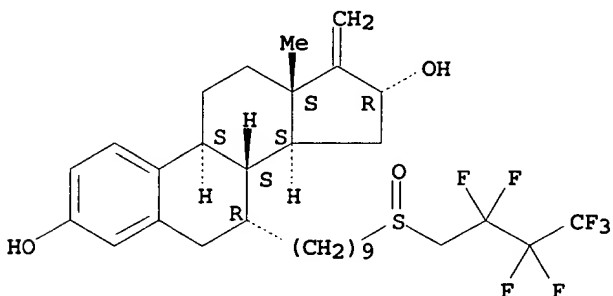
Absolute stereochemistry.



RN 862701-38-0 HCAPLUS

CN Estradiol, 7-[9-[(2,2,3,3,4,4,4-heptafluorobutyl)sulfinyl]nonyl]-17-methylene-, (7 α ,16 α)- (9CI) (CA INDEX NAME)

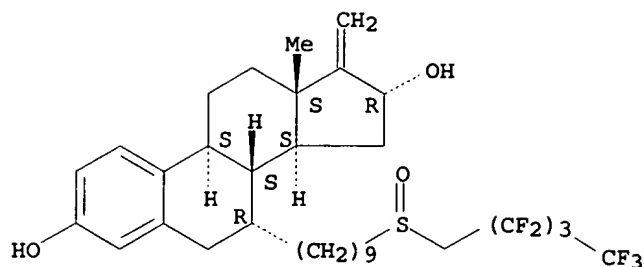
Absolute stereochemistry.



RN 862701-40-4 HCAPLUS

CN Estradiol, 17-methylene-7-[9-[(2,2,3,3,4,4,5,5,5-nonafluoropentyl)sulfinyl]nonyl]-, (7 α ,16 α)- (9CI) (CA INDEX NAME)

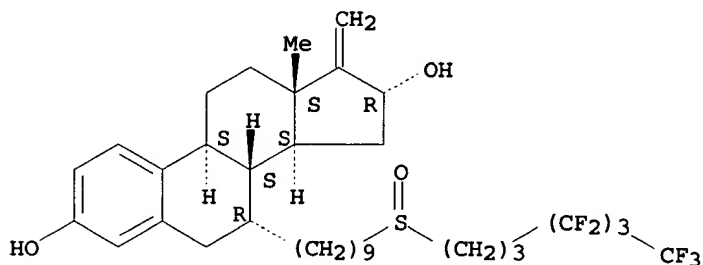
Absolute stereochemistry.



RN 862701-42-6 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 17-methylene-7-[9-[(4,4,5,5,6,6,7,7,7-nonafluoroheptyl)sulfinyl]nonyl]-, (7α,16α)- (9CI) (CA INDEX NAME)

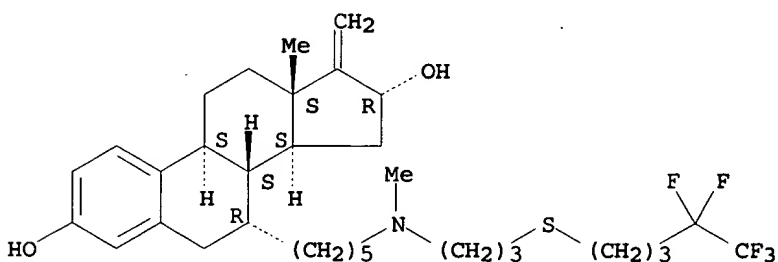
Absolute stereochemistry.



RN 862701-44-8 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 17-methylene-7-[5-[methyl[3-[(4,4,5,5,5-pentafluoropentyl)thio]propyl]amino]pentyl]-, (7α,16α)- (9CI) (CA INDEX NAME)

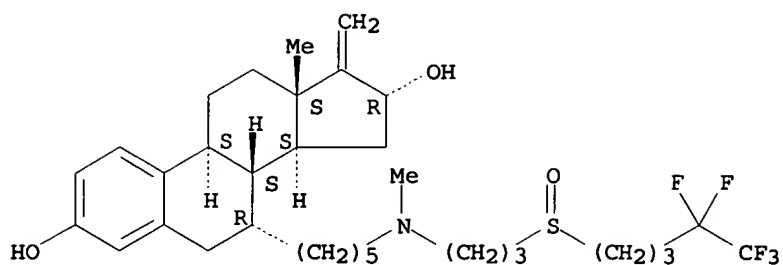
Absolute stereochemistry.



RN 862701-46-0 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 17-methylene-7-[5-[methyl[3-[(4,4,5,5,5-pentafluoropentyl)sulfinyl]propyl]amino]pentyl]-, (7α,16α)- (9CI) (CA INDEX NAME)

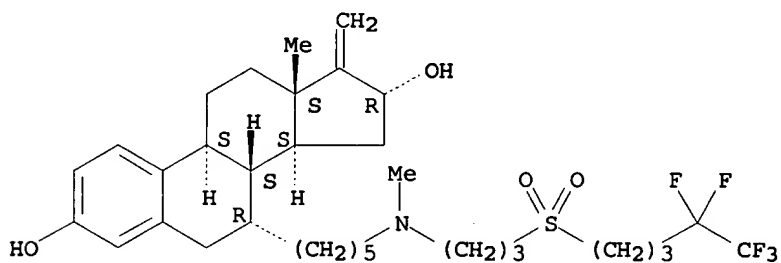
Absolute stereochemistry.



RN 862701-52-8 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 17-methylene-7-[5-[methyl 3-[(4,4,5,5,5-pentafluoropentyl)sulfonyl]propyl]amino]pentyl]-, (7α,16α)-(9CI) (CA INDEX NAME)

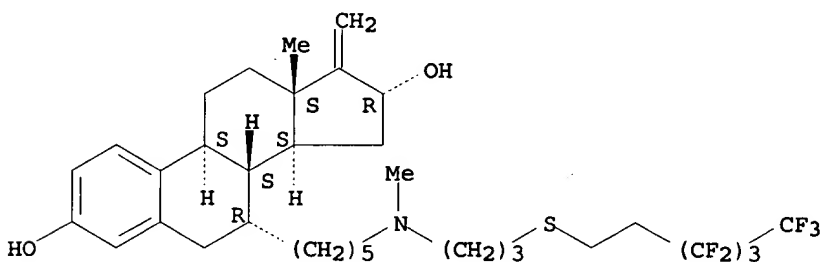
Absolute stereochemistry.



RN 862701-54-0 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 17-methylene-7-[5-[methyl 3-[(3,3,4,4,5,5,6,6,6-nonafluorohexyl)thio]propyl]amino]pentyl]-, (7α,16α)-(9CI) (CA INDEX NAME)

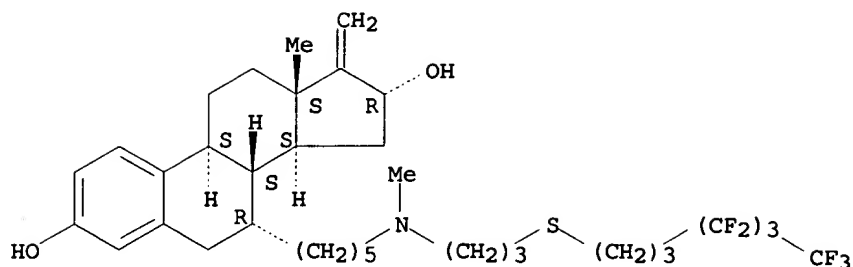
Absolute stereochemistry.



RN 862701-56-2 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 17-methylene-7-[5-[methyl 3-[(4,4,5,5,6,6,7,7,7-nonafluoroheptyl)thio]propyl]amino]pentyl]-, (7α,16α)-(9CI) (CA INDEX NAME)

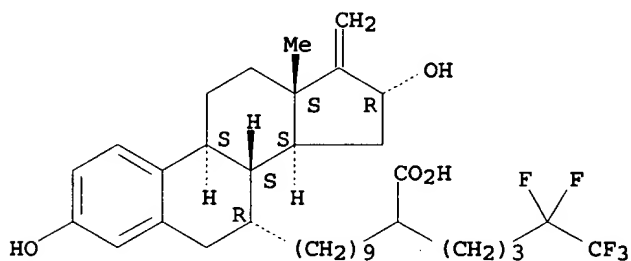
Absolute stereochemistry.



RN 862701-58-4 HCAPLUS

CN Estradiol-1,3,5(10)-triene-7-undecanoic acid, 3,16-dihydroxy-17-methylene- α -(4,4,5,5,5-pentafluoropentyl)-, (7 α ,16 α)- (9CI) (CA INDEX NAME)

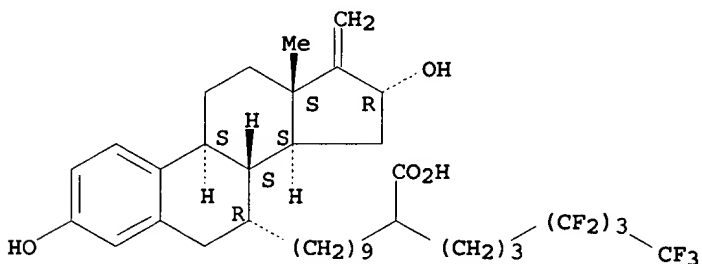
Absolute stereochemistry.



RN 862701-60-8 HCAPLUS

CN Estradiol-1,3,5(10)-triene-7-undecanoic acid, 3,16-dihydroxy-17-methylene- α -(4,4,5,5,6,6,7,7,7-nonafluoroheptyl)-, (7 α ,16 α)- (9CI) (CA INDEX NAME)

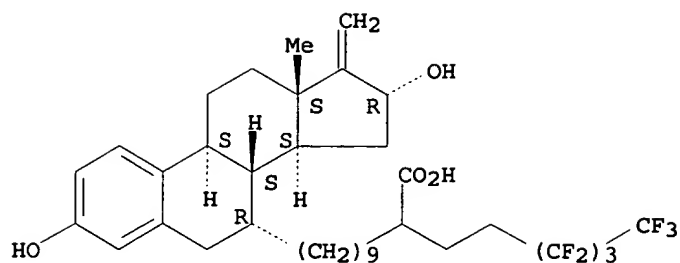
Absolute stereochemistry.



RN 862701-62-0 HCAPLUS

CN Estradiol-1,3,5(10)-triene-7-undecanoic acid, 3,16-dihydroxy-17-methylene- α -(3,3,4,4,5,5,6,6,6-nonafluorohexyl)-, (7 α ,16 α)- (9CI) (CA INDEX NAME)

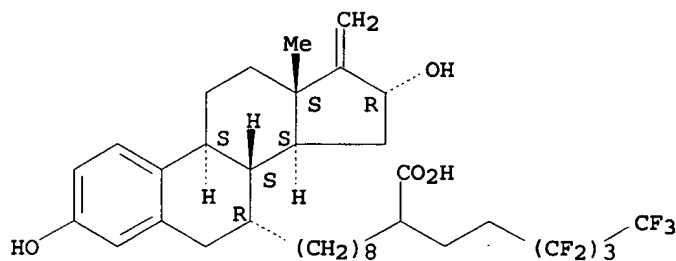
Absolute stereochemistry.



RN 862701-64-2 HCAPLUS

CN Estra-1,3,5(10)-triene-7-decanoic acid, 3,16-dihydroxy-17-methylene- α -(3,3,4,4,5,5,6,6,6-nonafluorohexyl)-, (7 α ,16 α)- (9CI) (CA INDEX NAME)

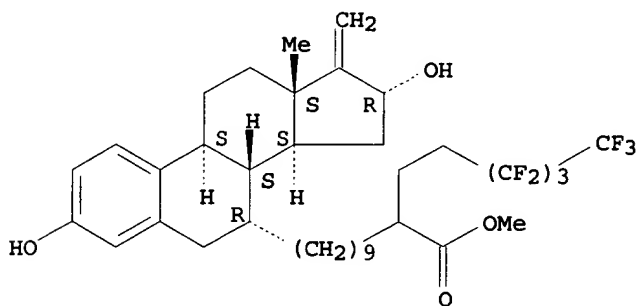
Absolute stereochemistry.



RN 862701-66-4 HCAPLUS

CN Estra-1,3,5(10)-triene-7-undecanoic acid, 3,16-dihydroxy-17-methylene- α -(3,3,4,4,5,5,6,6,6-nonafluorohexyl)-, methyl ester, (7 α ,16 α)- (9CI) (CA INDEX NAME)

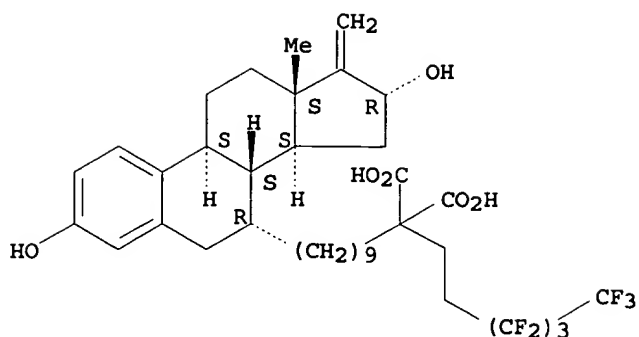
Absolute stereochemistry.



RN 862701-68-6 HCAPLUS

CN Propanedioic acid, [9-[(7 α ,16 α)-3,16-dihydroxy-17-methyleneestra-1,3,5(10)-trien-7-yl]nonyl] (3,3,4,4,5,5,6,6,6-nonafluorohexyl)- (9CI) (CA INDEX NAME)

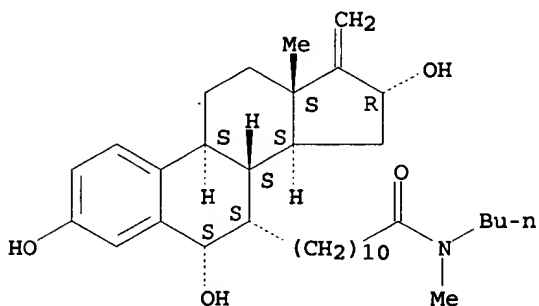
Absolute stereochemistry.



RN 862701-69-7 HCAPLUS

CN Estra-1,3,5(10)-triene-7-undecanamide, N-butyl-3,6,16-trihydroxy-N-methyl-17-methylene-, (6 α ,7 α ,16 α)- (9CI) (CA INDEX NAME)

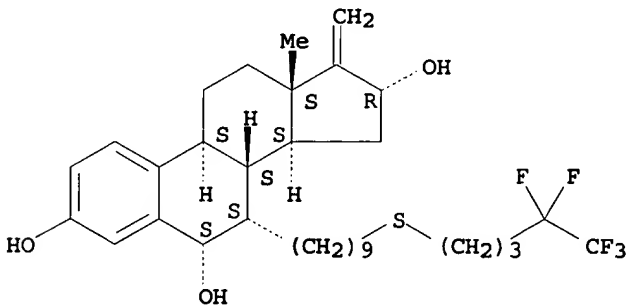
Absolute stereochemistry.



RN 862701-71-1 HCAPLUS

CN Estra-1,3,5(10)-triene-3,6,16-triol, 17-methylene-7-[9-[(4,4,5,5,5-pentafluoropentyl)thio]nonyl]-, (6 α ,7 α ,16 α)- (9CI) (CA INDEX NAME)

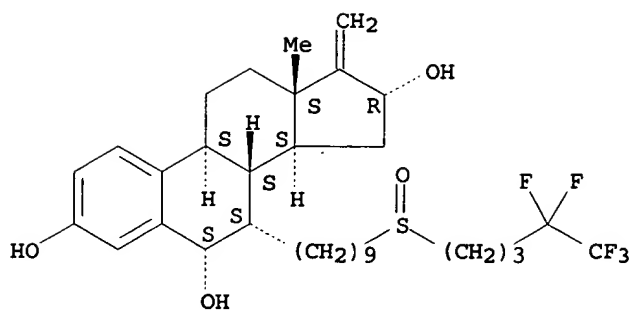
Absolute stereochemistry.



RN 862701-73-3 HCAPLUS

CN Estra-1,3,5(10)-triene-3,6,16-triol, 17-methylene-7-[9-[(4,4,5,5,5-pentafluoropentyl)sulfinyl]nonyl]-, (6 α ,7 α ,16 α)- (9CI) (CA INDEX NAME)

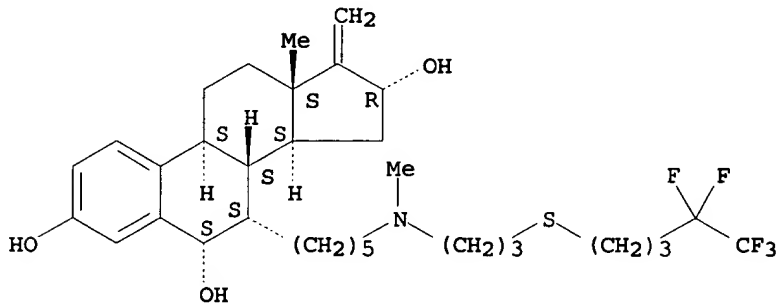
Absolute stereochemistry.



RN 862701-77-7 HCAPLUS

CN Estra-1,3,5(10)-triene-3,6,16-triol, 17-methylene-7-[5-[methyl[3-[(4,4,5,5,5-pentafluoropentyl)thio]propyl]amino]pentyl]-, (6 α ,7 α ,16 α)- (9CI) (CA INDEX NAME)

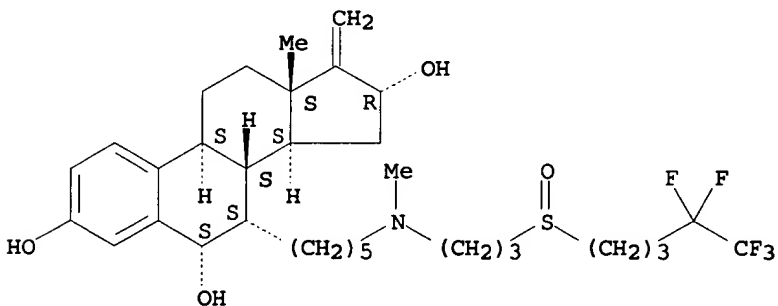
Absolute stereochemistry.



RN 862701-81-3 HCAPLUS

CN Estra-1,3,5(10)-triene-3,6,16-triol, 17-methylene-7-[5-[methyl[3-[(4,4,5,5,5-pentafluoropentyl)sulfinyl]propyl]amino]pentyl]-, (6 α ,7 α ,16 α)- (9CI) (CA INDEX NAME)

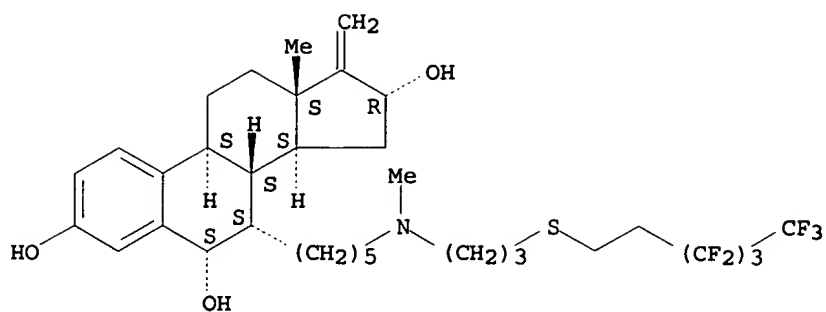
Absolute stereochemistry.



RN 862701-83-5 HCAPLUS

CN Estra-1,3,5(10)-triene-3,6,16-triol, 17-methylene-7-[5-[methyl[3-[(3,3,4,4,5,5,6,6,6-nonafluorohexyl)thio]propyl]amino]pentyl]-, (6 α ,7 α ,16 α)- (9CI) (CA INDEX NAME)

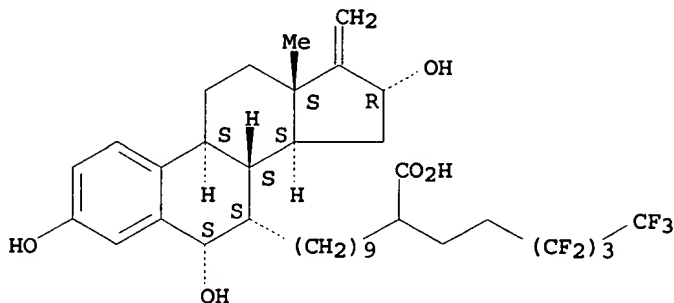
Absolute stereochemistry.



RN 862701-85-7 HCAPLUS

CN Estra-1,3,5(10)-triene-7-undecanoic acid, 3,6,16-trihydroxy-17-methylene- α -(3,3,4,4,5,5,6,6,6-nonafluorohexyl)-, (6 α ,7 α ,16 α)- (9CI) (CA INDEX NAME)

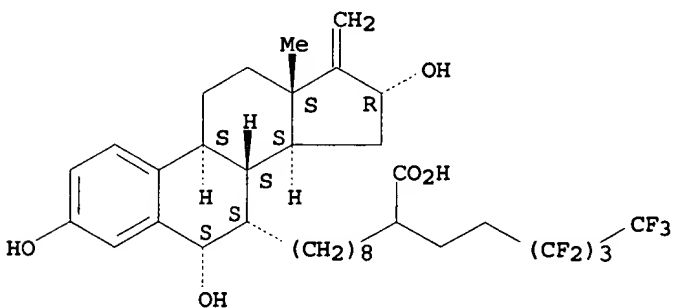
Absolute stereochemistry.



RN 862701-87-9 HCAPLUS

CN Estra-1,3,5(10)-triene-7-decanoic acid, 3,6,16-trihydroxy-17-methylene- α -(3,3,4,4,5,5,6,6,6-nonafluorohexyl)-, (6 α ,7 α ,16 α)- (9CI) (CA INDEX NAME)

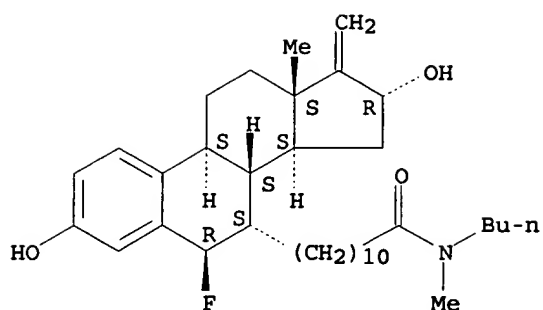
Absolute stereochemistry.



RN 862701-89-1 HCAPLUS

CN Estra-1,3,5(10)-triene-7-undecanamide, N-butyl-6-fluoro-3,16-dihydroxy-N-methyl-17-methylene-, (6 β ,7 α ,16 α)- (9CI) (CA INDEX NAME)

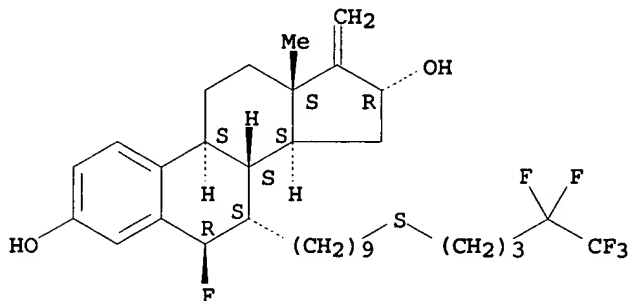
Absolute stereochemistry.



RN 862701-91-5 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 6-fluoro-17-methylene-7-[9-[(4,4,5,5,5-pentafluoropentyl)thio]nonyl]-, (6β,7α,16α)- (9CI) (CA INDEX NAME)

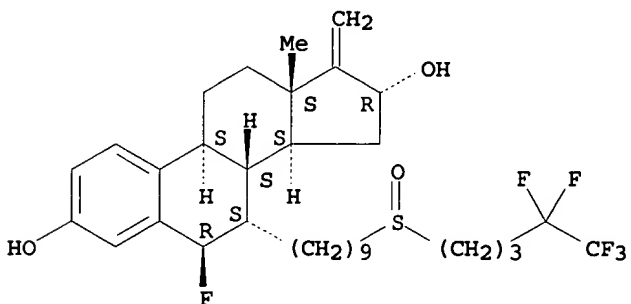
Absolute stereochemistry.



RN 862701-93-7 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 6-fluoro-17-methylene-7-[9-[(4,4,5,5,5-pentafluoropentyl)sulfinyl]nonyl]-, (6β,7α,16α)- (9CI) (CA INDEX NAME)

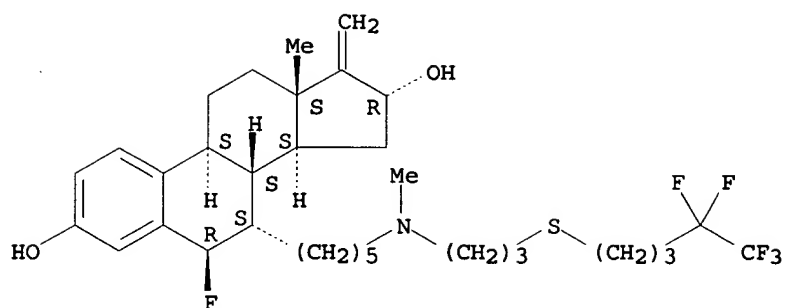
Absolute stereochemistry.



RN 862701-95-9 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 6-fluoro-17-methylene-7-[5-[methyl[3-[(4,4,5,5,5-pentafluoropentyl)thio]propyl]amino]pentyl]-, (6β,7α,16α)- (9CI) (CA INDEX NAME)

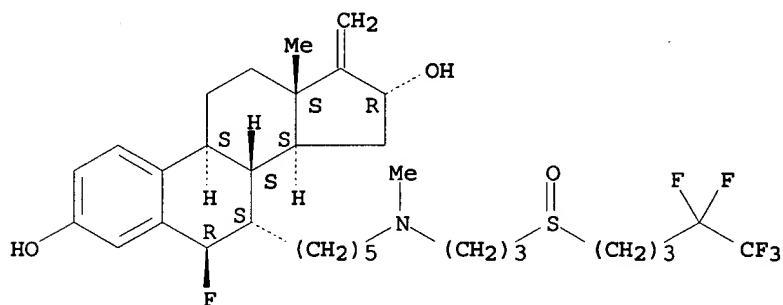
Absolute stereochemistry.



RN 862701-97-1 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 6-fluoro-17-methylene-7-[5-[methyl[3-[(4,4,5,5,5-pentafluoropentyl)sulfinyl]propyl]amino]pentyl]-, (6β,7α,16α)- (9CI) (CA INDEX NAME)

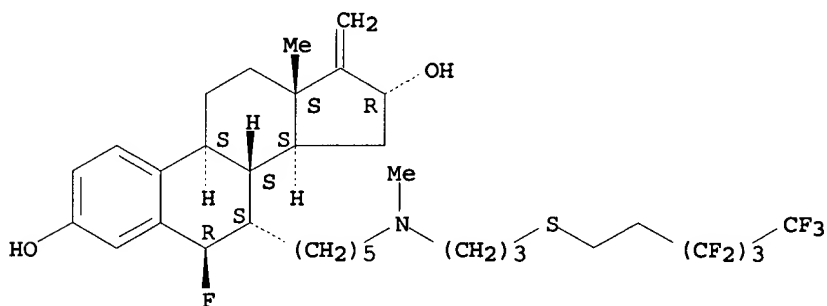
Absolute stereochemistry.



RN 862701-99-3 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 6-fluoro-17-methylene-7-[5-[methyl[3-[(3,3,4,4,5,5,6,6,6-nonafluorohexyl)thio]propyl]amino]pentyl]-, (6β,7α,16α)- (9CI) (CA INDEX NAME)

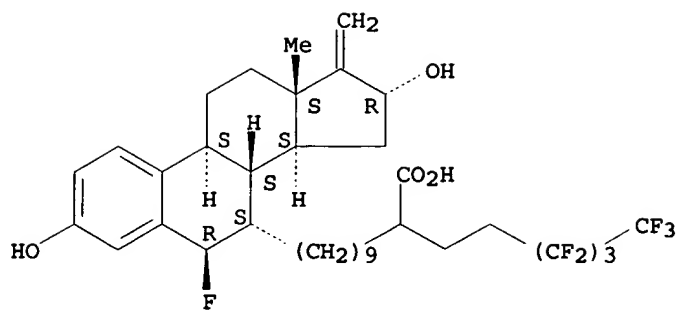
Absolute stereochemistry.



RN 862702-01-0 HCAPLUS

CN Estra-1,3,5(10)-triene-7-undecanoic acid, 6-fluoro-3,16-dihydroxy-17-methylene-α-(3,3,4,4,5,5,6,6,6-nonafluorohexyl)-, (6β,7α,16α)- (9CI) (CA INDEX NAME)

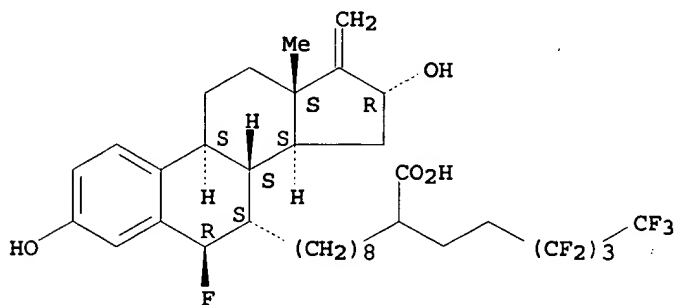
Absolute stereochemistry.



RN 862702-03-2 HCAPLUS

CN Estra-1,3,5(10)-triene-7-decanoic acid, 6-fluoro-3,16-dihydroxy-17-methylene- α -(3,3,4,4,5,5,6,6,6-nonafluorohexyl)-, (6 β ,7 α ,16 α)- (9CI) (CA INDEX NAME)

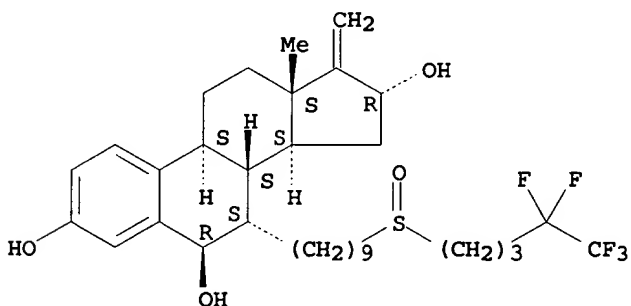
Absolute stereochemistry.



RN 862702-04-3 HCAPLUS

CN Estra-1,3,5(10)-triene-3,6,16-triol, 17-methylene-7-[9-[(4,4,5,5,5-pentafluoropentyl)sulfinyl]nonyl]-, (6 β ,7 α ,16 α)- (9CI) (CA INDEX NAME)

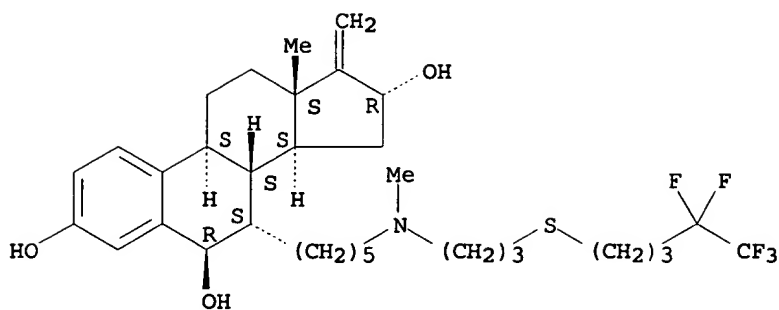
Absolute stereochemistry.



RN 862702-05-4 HCAPLUS

CN Estra-1,3,5(10)-triene-3,6,16-triol, 17-methylene-7-[5-[methyl[3-[(4,4,5,5,5-pentafluoropentyl)thio]propyl]amino]pentyl]-, (6 β ,7 α ,16 α)- (9CI) (CA INDEX NAME)

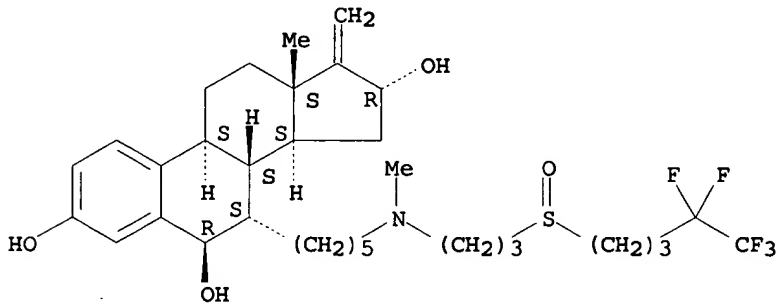
Absolute stereochemistry.



RN 862702-06-5 HCAPLUS

CN Estra-1,3,5(10)-triene-3,6,16-triol, 17-methylene-7-[5-[methyl[3-[(4,4,5,5,5-pentafluoropentyl)sulfinyl]propyl]amino]pentyl]-, (6β,7α,16α)- (9CI) (CA INDEX NAME)

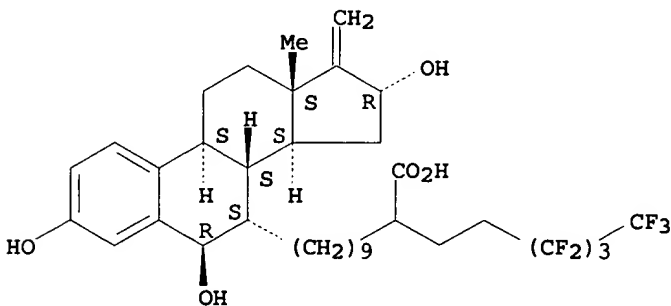
Absolute stereochemistry.



RN 862702-07-6 HCAPLUS

CN Estra-1,3,5(10)-triene-7-undecanoic acid, 3,6,16-trihydroxy-17-methylene-α-(3,3,4,4,5,5,6,6,6-nonafluorohexyl)-, (6β,7α,16α)- (9CI) (CA INDEX NAME)

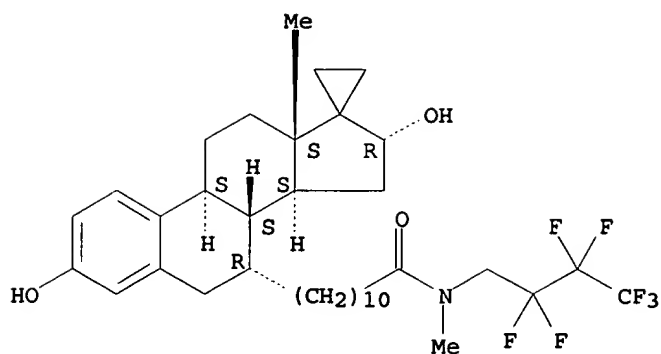
Absolute stereochemistry.



RN 862702-08-7 HCAPLUS

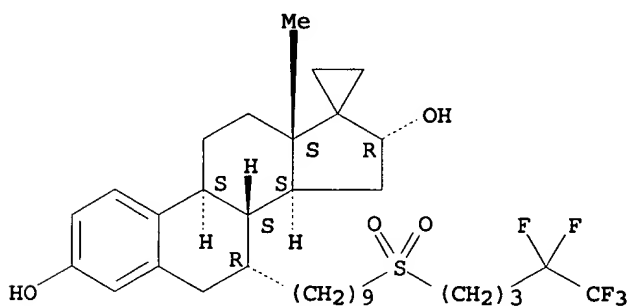
CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-7-undecanamide, N-(2,2,3,3,4,4,4-heptafluorobutyl)-3,16-dihydroxy-N-methyl-, (7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



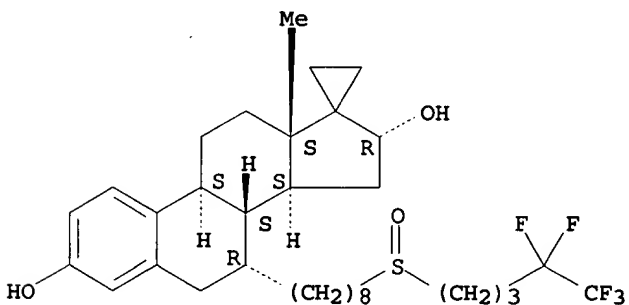
RN 862702-11-2 HCAPLUS
 CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-3,16-diol,
 7-[9-[(4,4,5,5,5-pentafluoropentyl)sulfonyl]nonyl]-,
 (7 α ,16 α)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



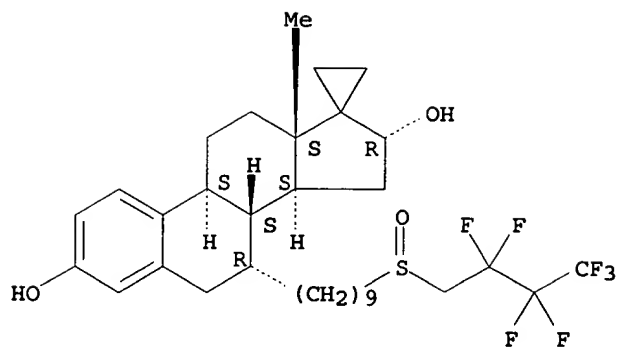
RN 862702-12-3 HCAPLUS
 CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-3,16-diol,
 7-[8-[(4,4,5,5,5-pentafluoropentyl)sulfinyl]octyl]-,
 (7 α ,16 α)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 862702-13-4 HCAPLUS
 CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-3,16-diol,
 7-[9-[(2,2,3,3,4,4,4-heptafluorobutyl)sulfinyl]nonyl]-,
 (7 α ,16 α)-(9CI) (CA INDEX NAME)

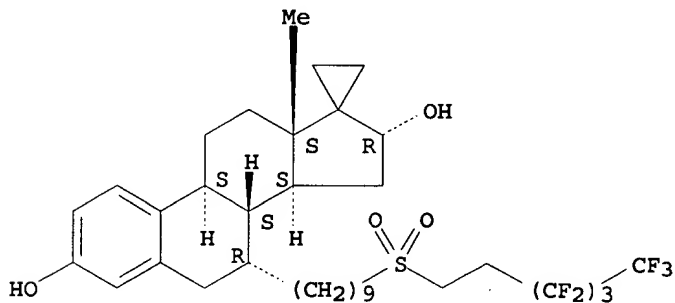
Absolute stereochemistry.



RN 862702-14-5 HCAPLUS

CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-3,16-diol,
7-[9-[(3,3,4,4,5,5,6,6,6-nonafluorohexyl)sulfonyl]nonyl]-,
(7 α ,16 α)-(9CI) (CA INDEX NAME)

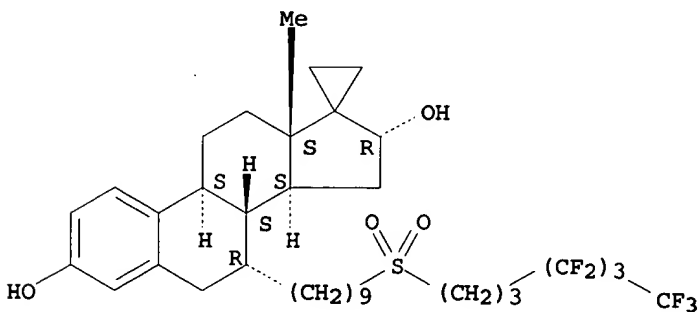
Absolute stereochemistry.



RN 862702-15-6 HCAPLUS

CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-3,16-diol,
7-[9-[(4,4,5,5,6,6,7,7,7-nonafluoroheptyl)sulfonyl]nonyl]-,
(7 α ,16 α)-(9CI) (CA INDEX NAME)

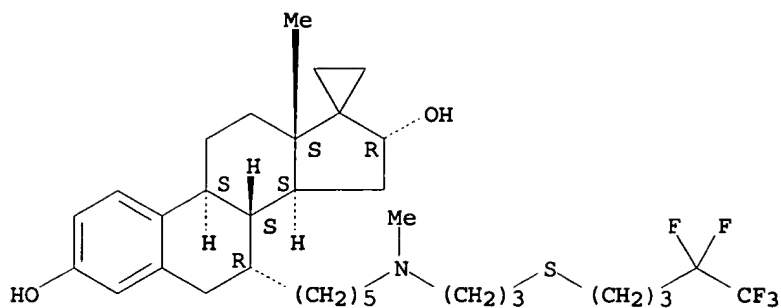
Absolute stereochemistry.



RN 862702-16-7 HCAPLUS

CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-3,16-diol,
7-[5-[methyl[3-[(4,4,5,5,5-pentafluoropentyl)thio]propyl]amino]pen
tyl]-, (7 α ,16 α)-(9CI) (CA INDEX NAME)

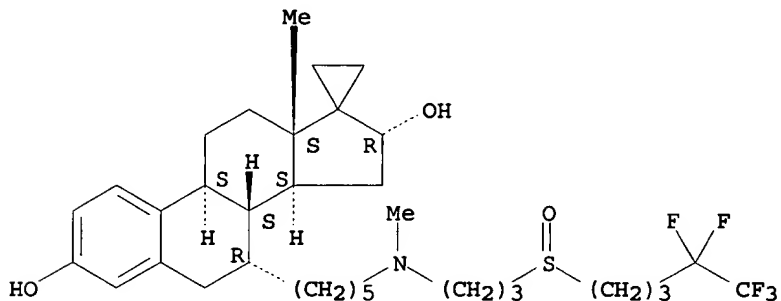
Absolute stereochemistry.



RN 862702-20-3 HCAPLUS

CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-3,16-diol,
7-[5-[methyl 3-[(4,4,5,5,5-pentafluoropentyl)sulfinyl]propyl]amino]
pentyl]-, (7 α ,16 α)- (9CI) (CA INDEX NAME)

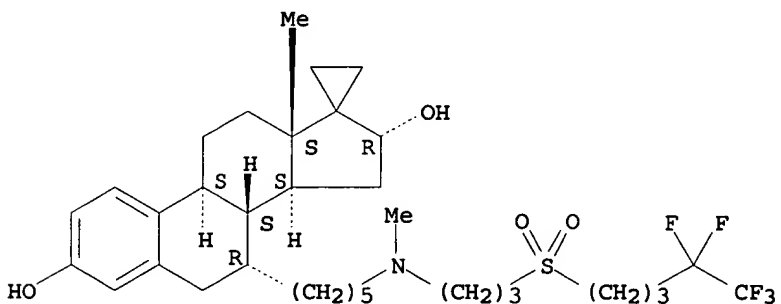
Absolute stereochemistry.



RN 862702-21-4 HCAPLUS

CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-3,16-diol,
7-[5-[methyl 3-[(4,4,5,5,5-pentafluoropentyl)sulfonyl]propyl]amino]
pentyl]-, (7 α ,16 α)- (9CI) (CA INDEX NAME)

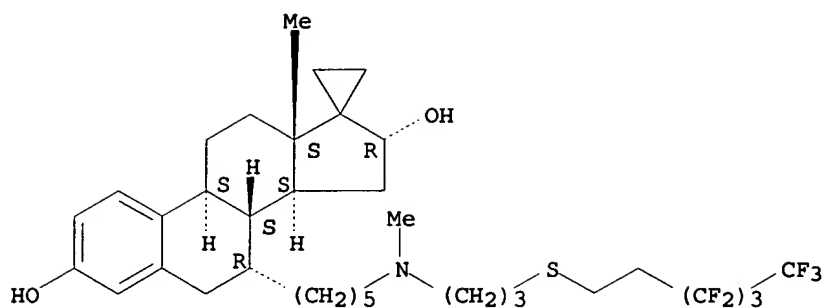
Absolute stereochemistry.



RN 862702-22-5 HCAPLUS

CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-3,16-diol,
7-[5-[methyl 3-[(3,3,4,4,5,5,6,6,6-nonafluorohexyl)thio]propyl]ami
no]pentyl]-, (7 α ,16 α)- (9CI) (CA INDEX NAME)

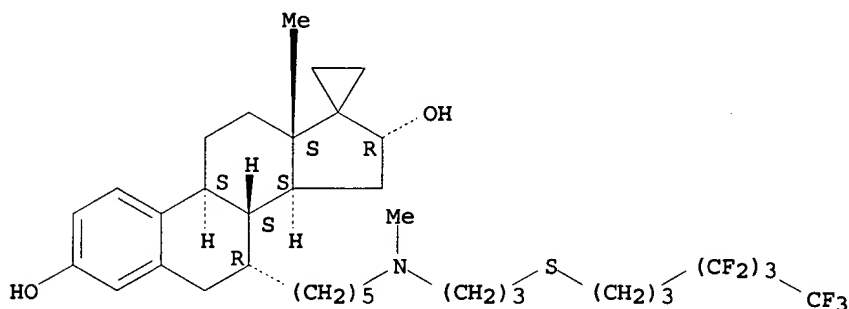
Absolute stereochemistry.



RN 862702-23-6 HCAPLUS

CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-3,16-diol,
7-[5-[methyl[3-[(4,4,5,5,6,6,7,7,7-nonafluoroheptyl)thio]propyl]amino]pentyl]-, (7 α ,16 α)- (9CI) (CA INDEX NAME)

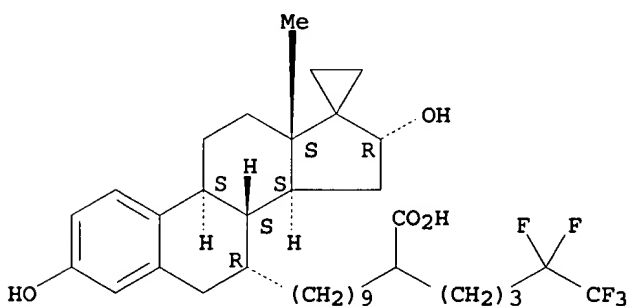
Absolute stereochemistry.



RN 862702-24-7 HCAPLUS

CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-7-undecanoic acid,
3,16-dihydroxy- α -(4,4,5,5,5-pentafluoropentyl)-, (7 α ,16 α)- (9CI) (CA INDEX NAME)

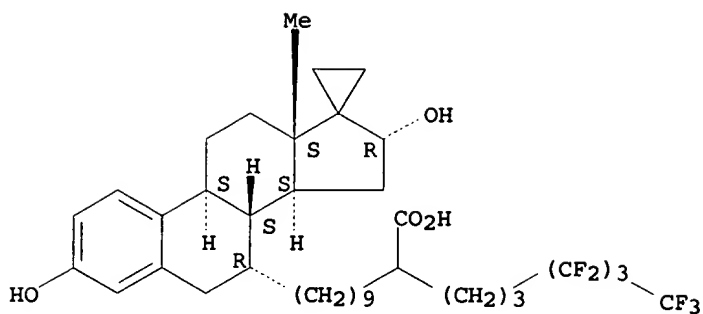
Absolute stereochemistry.



RN 862702-25-8 HCAPLUS

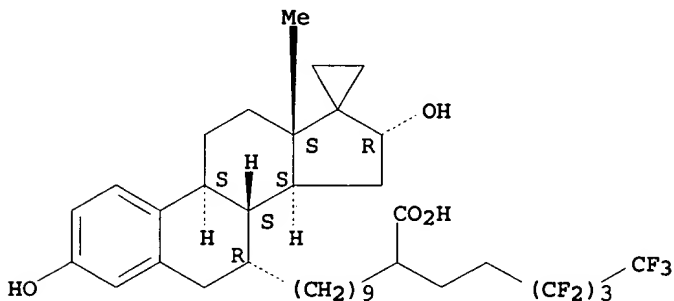
CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-7-undecanoic acid,
3,16-dihydroxy- α -(4,4,5,5,6,6,7,7,7-nonafluoroheptyl)-, (7 α ,16 α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



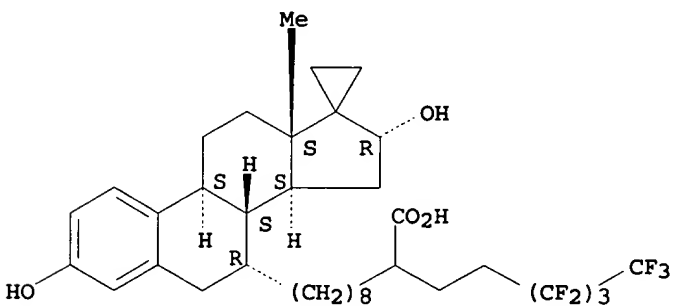
RN 862702-26-9 HCAPLUS
 CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-7-undecanoic acid,
 3,16-dihydroxy- α -(3,3,4,4,5,5,6,6,6-nonafluorohexyl)-,
 (7 α ,16 α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



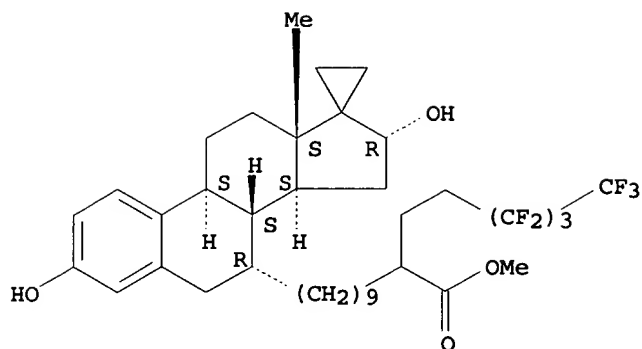
RN 862702-27-0 HCAPLUS
 CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-7-decanoic acid,
 3,16-dihydroxy- α -(3,3,4,4,5,5,6,6,6-nonafluorohexyl)-,
 (7 α ,16 α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 862702-28-1 HCAPLUS
 CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-7-undecanoic acid,
 3,16-dihydroxy- α -(3,3,4,4,5,5,6,6,6-nonafluorohexyl)-,
 methyl ester, (7 α ,16 α)- (9CI) (CA INDEX NAME)

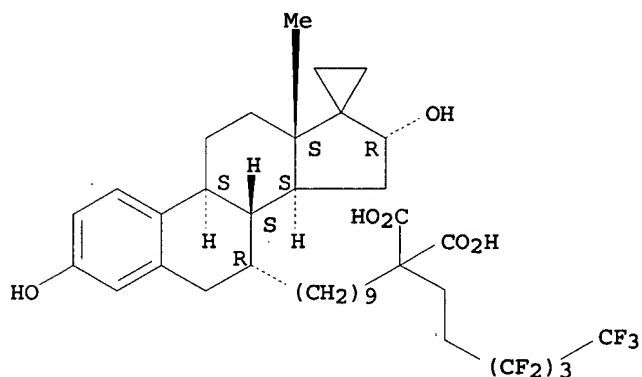
Absolute stereochemistry.



RN 862702-29-2 HCAPLUS

CN Propanedioic acid, [9-[(7 α ,16 α)-3,16-dihydroxy-17,21-cyclo-19-norpregna-1,3,5(10)-trien-7-yl]nonyl] (3,3,4,4,5,5,6,6,6-nonafluorohexyl)- (9CI) (CA INDEX NAME)

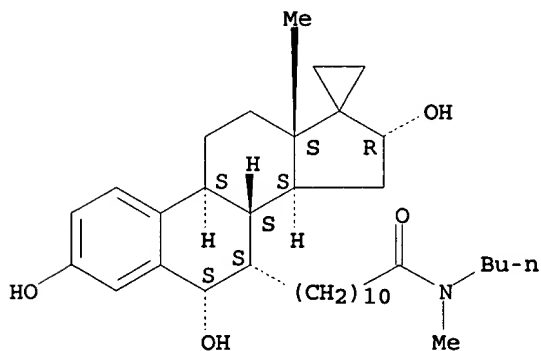
Absolute stereochemistry.



RN 862702-30-5 HCAPLUS

CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-7-undecanamide, N-butyl-3,6,16-trihydroxy-N-methyl-, (6 α ,7 α ,16 α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

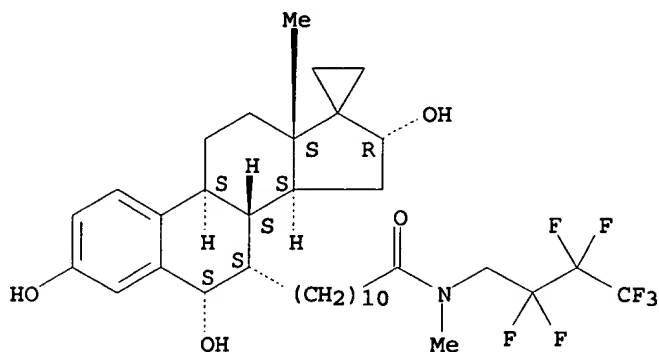


RN 862702-31-6 HCAPLUS

CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-7-undecanamide,

N-(2,2,3,3,4,4,4-heptafluorobutyl)-3,6,16-trihydroxy-N-methyl-,
(6 α ,7 α ,16 α)- (9CI) (CA INDEX NAME)

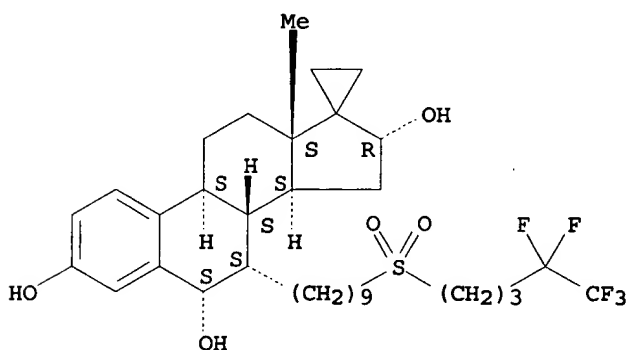
Absolute stereochemistry.



RN 862702-33-8 HCAPLUS

CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-3,6,16-triol,
7-[9-[(4,4,5,5,5-pentafluoropentyl)sulfonyl]nonyl]-,
(6 α ,7 α ,16 α)- (9CI) (CA INDEX NAME)

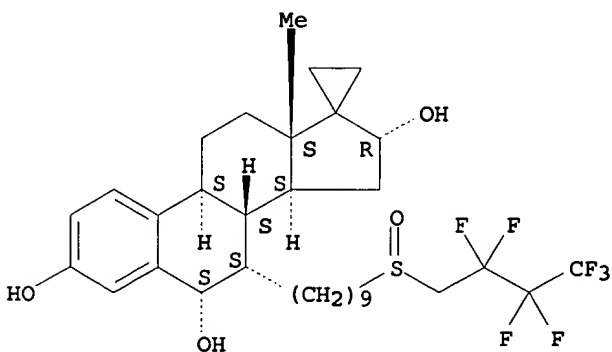
Absolute stereochemistry.



RN 862702-34-9 HCAPLUS

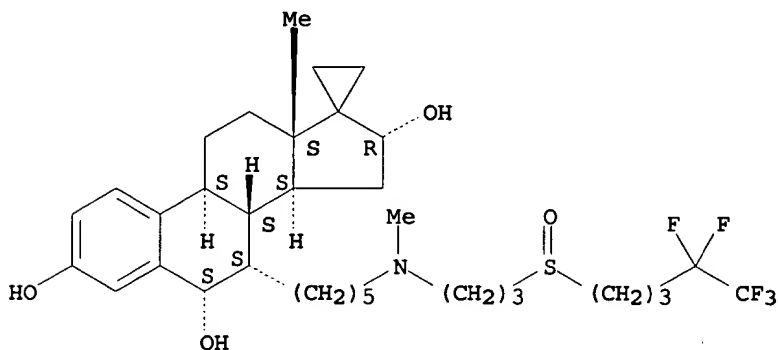
CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-3,6,16-triol,
7-[9-[(2,2,3,3,4,4,4-heptafluorobutyl)sulfonyl]nonyl]-,
(6 α ,7 α ,16 α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



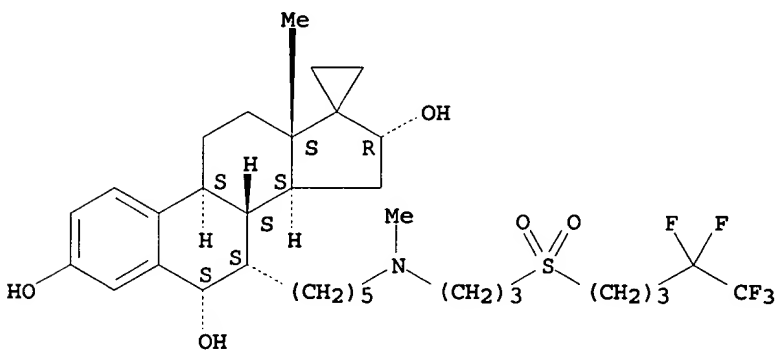
RN 862702-36-1 HCAPLUS
 CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-3,6,16-triol,
 7-[5-[methyl 3-[(4,4,5,5,5-pentafluoropentyl)sulfinyl]propyl]amino
]pentyl]-, (6 α ,7 α ,16 α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



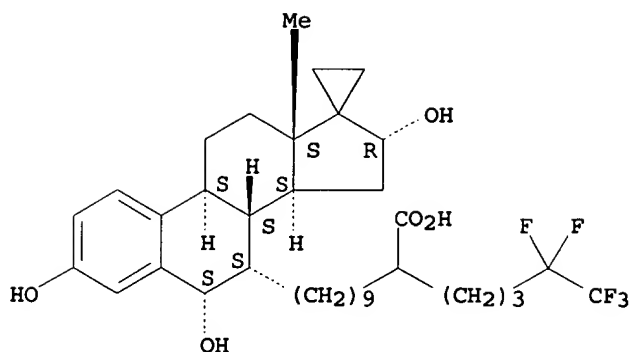
RN 862702-37-2 HCAPLUS
 CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-3,6,16-triol,
 7-[5-[methyl 3-[(4,4,5,5,5-pentafluoropentyl)sulfonyl]propyl]amino
]pentyl]-, (6 α ,7 α ,16 α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 862702-38-3 HCAPLUS
 CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-7-undecanoic acid,
 3,6,16-trihydroxy- α -(4,4,5,5,5-pentafluoropentyl)-,
 (6 α ,7 α ,16 α)- (9CI) (CA INDEX NAME)

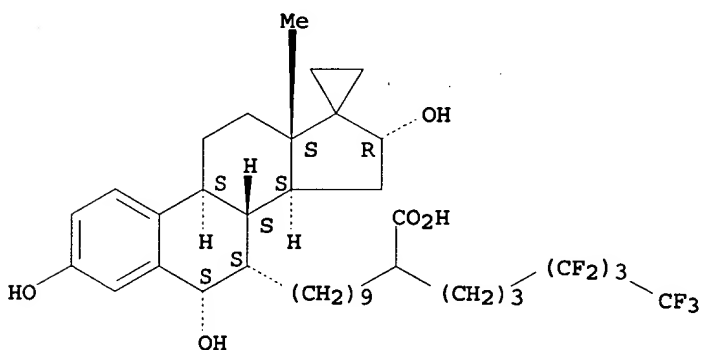
Absolute stereochemistry.



RN 862702-39-4 HCAPLUS

CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-7-undecanoic acid,
3,6,16-trihydroxy- α -(4,4,5,5,6,6,7,7,7-nonafluoroheptyl)-,
(6 α ,7 α ,16 α)- (9CI) (CA INDEX NAME)

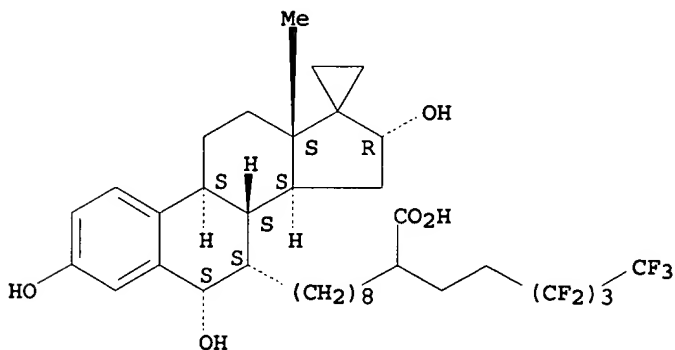
Absolute stereochemistry.



RN 862702-40-7 HCAPLUS

CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-7-decanoic acid,
3,6,16-trihydroxy- α -(3,3,4,4,5,5,6,6,6-nonafluorohexyl)-,
(6 α ,7 α ,16 α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

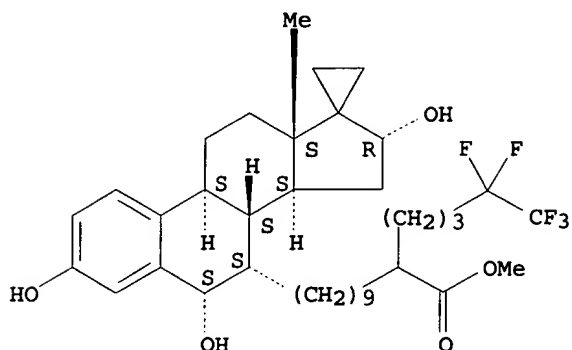


RN 862702-41-8 HCAPLUS

CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-7-undecanoic acid,
3,6,16-trihydroxy- α -(4,4,5,5,5-pentafluoropentyl)-, methyl

ester, (6 α ,7 α ,16 α)- (9CI) (CA INDEX NAME)

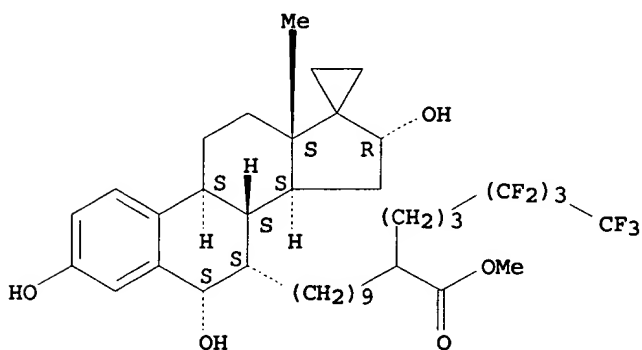
Absolute stereochemistry.



RN 862702-42-9 HCAPLUS

CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-7-undecanoic acid,
3,6,16-trihydroxy- α -(4,4,5,5,6,6,7,7,7-nonafluoroheptyl)-,
methyl ester, (6 α ,7 α ,16 α)- (9CI) (CA INDEX
NAME)

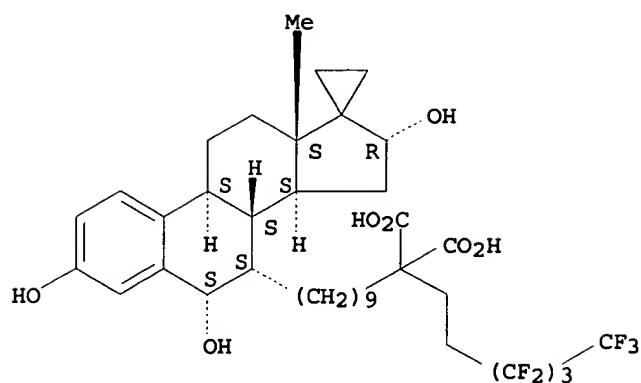
Absolute stereochemistry.



RN 862702-43-0 HCAPLUS

CN Propanedioic acid, (3,3,4,4,5,5,6,6,6-nonafluorohexyl) [9-
[(6 α ,7 α ,16 α)-3,6,16-trihydroxy-17,21-cyclo-19-
norpregna-1,3,5(10)-trien-7-yl]nonyl]- (9CI) (CA INDEX NAME)

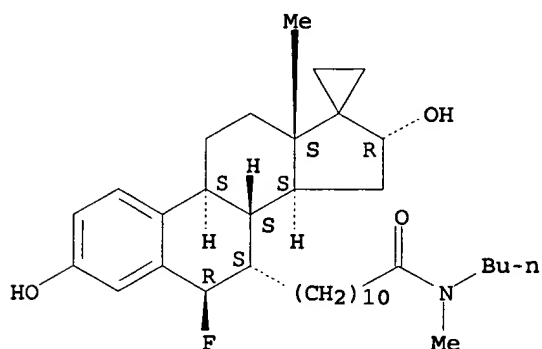
Absolute stereochemistry.



RN 862702-44-1 HCAPLUS

CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-7-undecanamide,
N-butyl-6-fluoro-3,16-dihydroxy-N-methyl-,
(6β,7α,16α)- (9CI) (CA INDEX NAME)

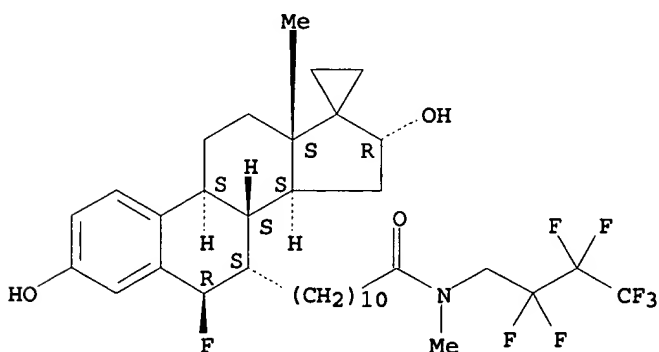
Absolute stereochemistry.



RN 862702-45-2 HCAPLUS

CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-7-undecanamide,
6-fluoro-N-(2,2,3,3,4,4,4-heptafluorobutyl)-3,16-dihydroxy-N-
methyl-, (6β,7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

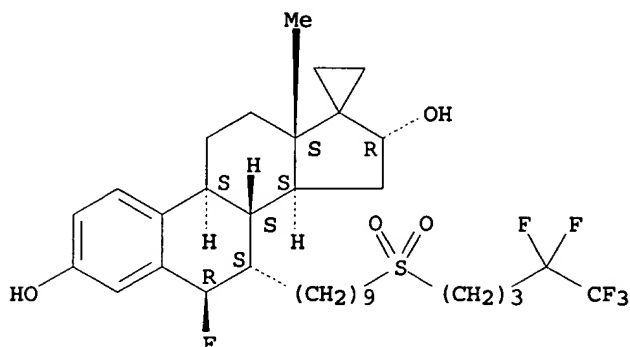


RN 862702-47-4 HCAPLUS

CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-3,16-diol,
6-fluoro-N-(2,2,3,3,4,4,4-heptafluorobutyl)-3,16-dihydroxy-N-
methyl-, (6β,7α,16α)- (9CI) (CA INDEX NAME)

6-fluoro-7-[9-[(4,4,5,5,5-pentafluoropentyl)sulfonyl]nonyl]-,
(6 β ,7 α ,16 α)- (9CI) (CA INDEX NAME)

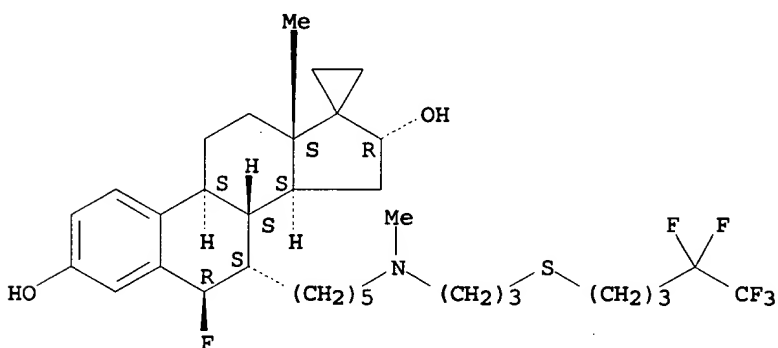
Absolute stereochemistry.



RN 862702-48-5 HCAPLUS

CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-3,16-diol,
6-fluoro-7-[5-[methyl[3-[(4,4,5,5,5-pentafluoropentyl)thio]propyl]
aminopentyl]-, (6 β ,7 α ,16 α)- (9CI) (CA INDEX
NAME)

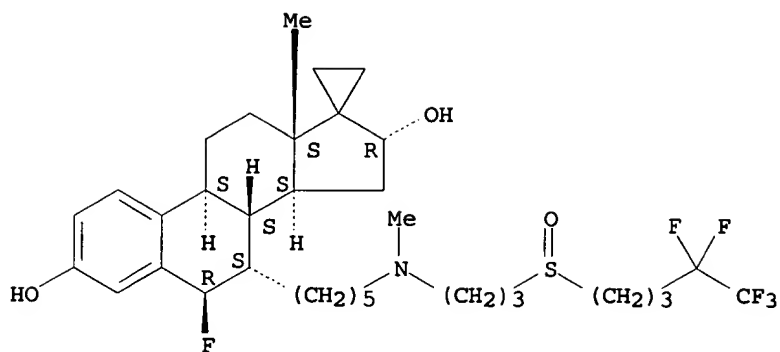
Absolute stereochemistry.



RN 862702-50-9 HCAPLUS

CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-3,16-diol,
6-fluoro-7-[5-[methyl[3-[(4,4,5,5,5-pentafluoropentyl)sulfinyl]pro
pyl]aminopentyl]-, (6 β ,7 α ,16 α)- (9CI) (CA INDEX
NAME)

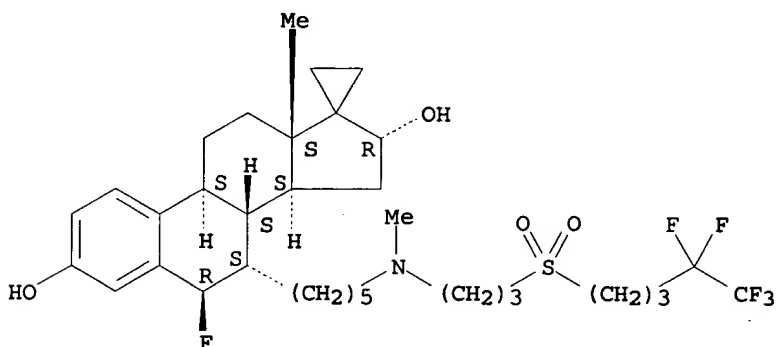
Absolute stereochemistry.



RN 862702-51-0 HCAPLUS

CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-3,16-diol,
6-fluoro-7-[5-[methyl[3-[(4,4,5,5,5-pentafluoropentyl)sulfonyl]pro-
pyl]aminopentyl]-, (6β,7α,16α)- (9CI) (CA INDEX
NAME)

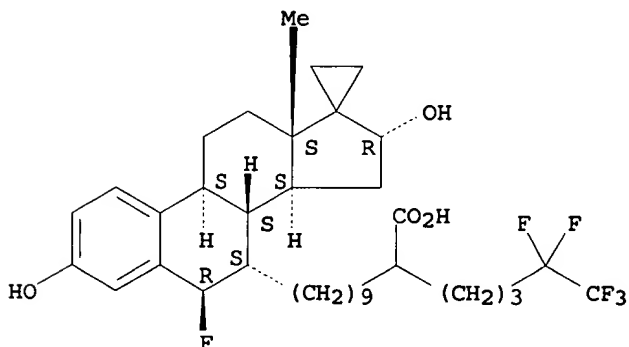
Absolute stereochemistry.



RN 862702-52-1 HCAPLUS

CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-7-undecanoic acid,
6-fluoro-3,16-dihydroxy-α-(4,4,5,5,5-pentafluoropentyl)-,
(6β,7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

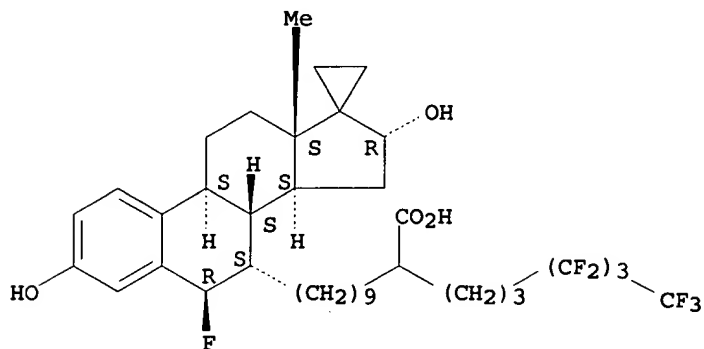


RN 862702-53-2 HCAPLUS

CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-7-undecanoic acid,

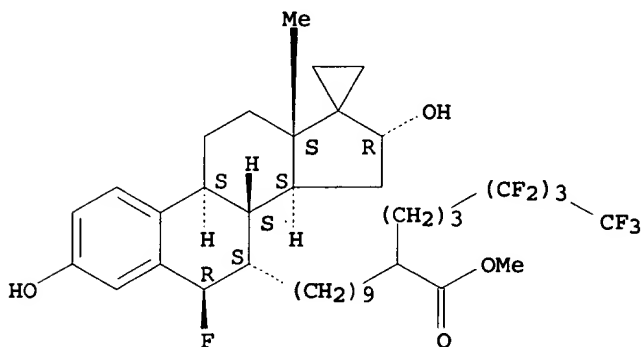
6-fluoro-3,16-dihydroxy- α -(4,4,5,5,6,6,7,7,7-nonafluoroheptyl)-, (6 β ,7 α ,16 α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



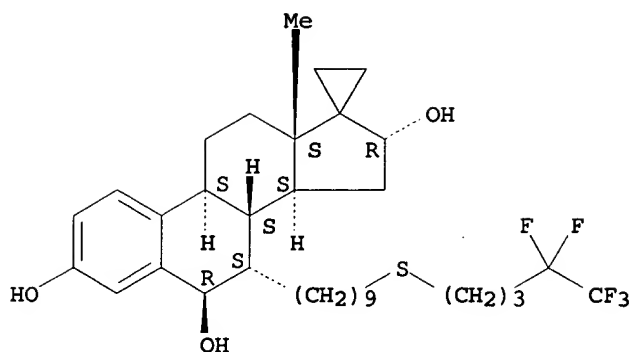
RN 862702-54-3 HCAPLUS
 CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-7-undecanoic acid, 6-fluoro-3,16-dihydroxy- α -(4,4,5,5,6,6,7,7,7-nonafluoroheptyl)-, methyl ester, (6 β ,7 α ,16 α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 862702-55-4 HCAPLUS
 CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-3,6,16-triol, 7-[9-[(4,4,5,5,5-pentafluoropentyl)thio]nonyl]-, (6 β ,7 α ,16 α)- (9CI) (CA INDEX NAME)

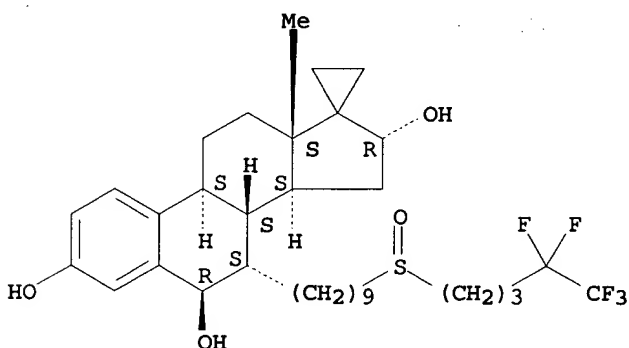
Absolute stereochemistry.



RN 862702-56-5 HCAPLUS

CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-3,6,16-triol,
7-[9-[(4,4,5,5,5-pentafluoropentyl)sulfinyl]nonyl]-,
(6 β ,7 α ,16 α)- (9CI) (CA INDEX NAME)

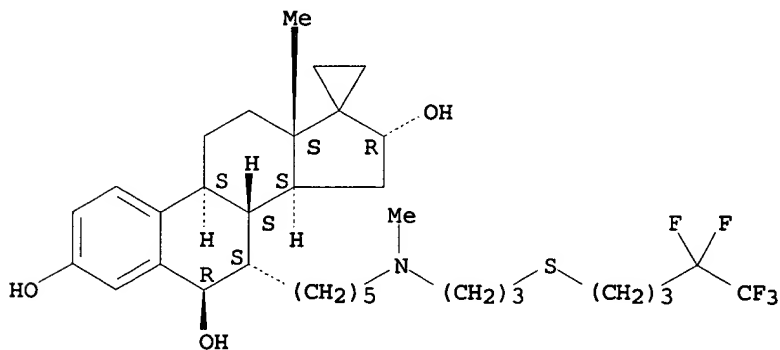
Absolute stereochemistry.



RN 862702-57-6 HCAPLUS

CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-3,6,16-triol,
7-[5-[methyl 3-[(4,4,5,5,5-pentafluoropentyl)thio]propyl]aminopentyl]-,
(6 β ,7 α ,16 α)- (9CI) (CA INDEX NAME)

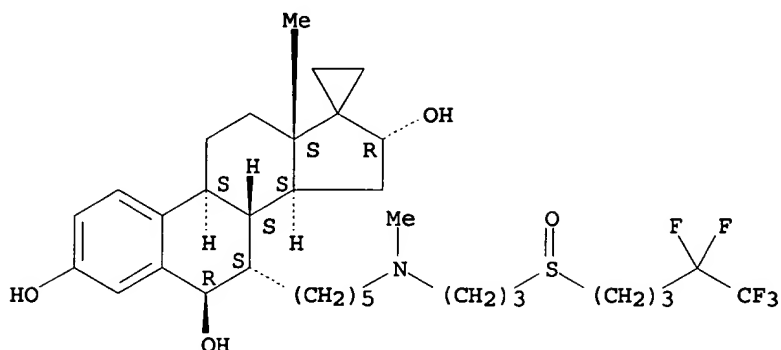
Absolute stereochemistry.



RN 862702-59-8 HCAPLUS

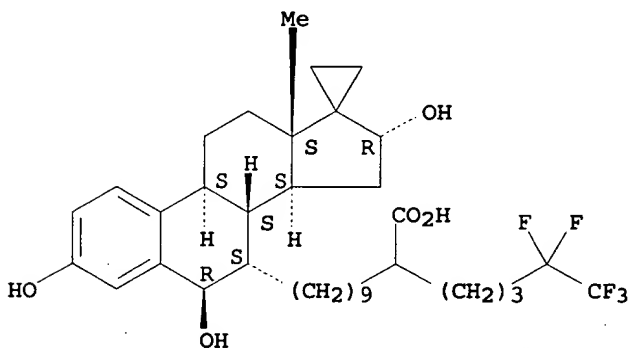
CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-3,6,16-triol,
7-[5-[methyl 3-[(4,4,5,5,5-pentafluoropentyl)sulfinyl]propyl]amino]-

Absolute stereochemistry.



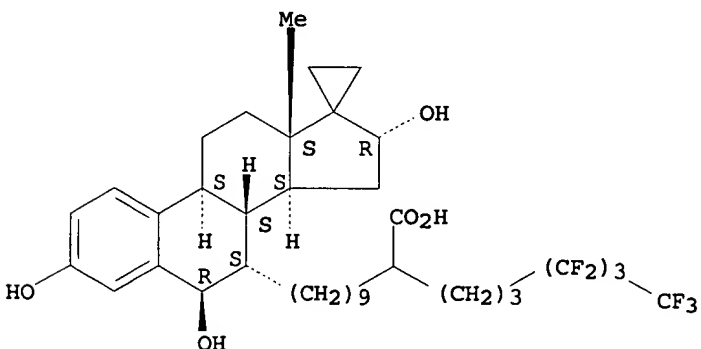
17,21-Cyclo-19-norpregna-1,3,5(10)-triene-7-undecanoic acid,
3,6,16-trihydroxy- α -(4,4,5,5,5-pentafluoropentyl)-,
(6 β ,7 α ,16 α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-7-undecanoic acid,
3,6,16-trihydroxy- α -(4,4,5,5,6,6,7,7,7-nonafluoroheptyl)-,
(6 β ,7 α ,16 α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

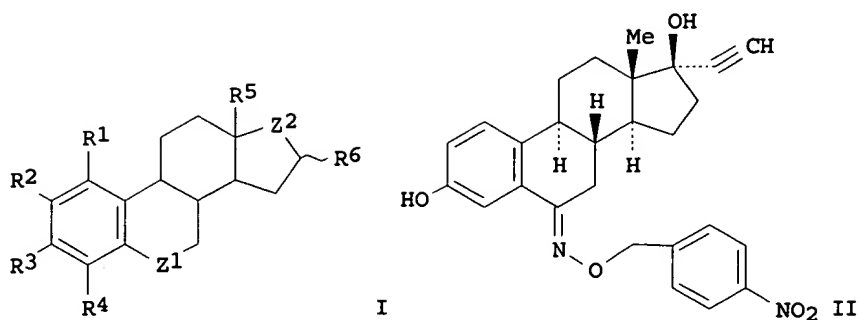


IC ICM C07J003-00
CC 32-3 (Steroids)
Section cross-reference(s): 2, 63
ST estrogen alkylene hydroxy prepn antiestrogen antitumor
IT Mammary gland, neoplasm
(estrogen dependent; preparation of antiestrogenic
17-alkylene-16 α -hydroxyestratrienes for cancer treatment)
IT Estrogens
RL: PAC (Pharmacological activity); SPN (Synthetic preparation);
THU (Therapeutic use); BIOL (Biological study); PREP
(Preparation); USES (Uses)
(preparation of antiestrogenic 17-alkylene-16 α -
hydroxyestratrienes for cancer treatment)
IT 862700-33-2P 862700-35-4P 862700-36-5P
862700-40-1P 862700-44-5P 862700-47-8P
862700-49-0P 862700-51-4P 862700-53-6P
862700-55-8P 862700-57-0P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic
preparation); THU (Therapeutic use); BIOL (Biological
study); PREP (Preparation); RACT (Reactant or reagent); USES
(Uses)
(preparation of antiestrogenic 17-alkylene-16 α -
hydroxyestratrienes for cancer treatment)
IT 862700-38-7P 862700-42-3P 862700-46-7P
862700-48-9P 862700-50-3P 862700-52-5P
862700-54-7P 862700-56-9P 862700-59-2P
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862702-54-3P 862702-55-4P 862702-56-5P
862702-57-6P 862702-59-8P 862702-60-1P
862702-61-2P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation);
THU (Therapeutic use); BIOL (Biological study); PREP
(Preparation); USES (Uses)
(preparation of antiestrogenic 17-alkylene-16 α -
hydroxyestratrienes for cancer treatment)

L53 ANSWER 3 OF 16 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:1016067 HCAPLUS
 DOCUMENT NUMBER: 141:424344
 TITLE: Preparation of estratriene derivatives for
 treating asthma and airway diseases
 INVENTOR(S): Stewart, Alastair George
 PATENT ASSIGNEE(S): Cryptopharma Pty. Ltd., Australia; McAllister,
 David James; Lambert, John Nicholas
 SOURCE: PCT Int. Appl., 219 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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WO 2004101595	A1	20041125	WO 2004-AU630	2004 0513
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	CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG,			
	ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP,			
	KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD,			
	MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL,			
	PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR,			
	TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM,			
	ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH,			
	CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU,			
	MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI,			
	CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
CA 2525651	AA	20041125	CA 2004-2525651	2004 0513
EP 1625143	A1	20060215	EP 2004-732553	2004 0513
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE,			
	MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK			
PRIORITY APPLN. INFO.:			US 2003-470379P	2003 0513
			WO 2004-AU630	W 2004 0513
OTHER SOURCE(S):	MARPAT 141:424344			
GI				



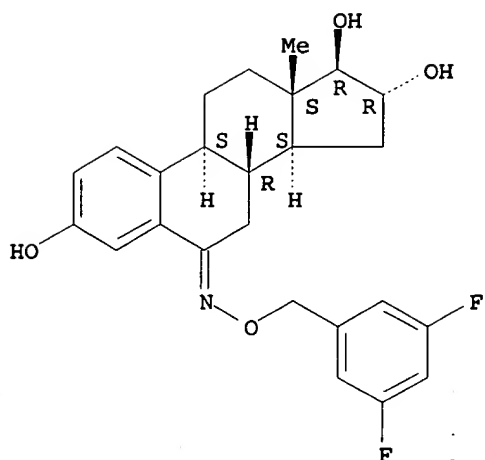
AB The present invention relates to preparation of estratriene derivs., such as I [R1, R4 = H, Ra, Rcrd, CN, NO2, halo, OH, ORa, OCORa; R2 = ORb, (Rc)nARb, H, CH:NOH, OH, SRb, Rb, CN, Rcrd, halo; n = 0-1; R3 = OH, ORa, RCORb, H; R5 = Me; R6 = H, OH, ORb, halo; Z1 = A, CO, CHOH, C:NOH, C:NORb, C(Rb)NRb2, CRb2, C:NNH2, C:NNRb2, O, NRb, CRbRCORb, CRbre, CRbNRbRe, C:N-ester-Ra; Z2 = A, CO, CHOH, C:NOH, C:NORb, C(Rb)ORb, CRbRCORb, CHNRb2, CH-halo, C:N-ester-Ra; A = C:NOX, C:NORCX, C:NNHRCX, C:NNHX, C:N-ester-X; X = substituted aromatic; Ra = alkyl, cycloalkyl, alkenyl, alkynyl, aralkyl, aralkenyl, aralkynyl; Rb = H, alkyl, cycloalkyl, alkenyl, alkynyl, aralkyl, aralkenyl, aralkynyl; RC = alkylene, alkenylene, alkynylene; Rd = OH, NH2, halo, CF3, CN, CO2Ra, SRb; Re = acyl], and methods for modulating mesenchymal cell function, for instance smooth muscle and fibroblast proliferation or cytokine expression, and for treating conditions associated with mesenchymal cell function, for instance airway hyperresponsiveness associated with asthma. The prepared compds. also suppress inflammation. Thus, estratriene derivative II was prepared which at 3µM reduced basic fibroblast growth factor (bFGF) induced proliferation by 93 ± 4 %. In a preferred embodiment, the estratriene derivs. include various derivs. of 2-methoxyestradiol having a substituted aromatic substituent in the 2-, 6- or 17- position.

IT 796848-26-5P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation);
THU (Therapeutic use); BIOL (Biological study); PREP
(Preparation); USES (Uses)
(preparation of estratriene derivs. for treating asthma and airway
diseases)

RN 796848-26-5 HCAPLUS

CN Estr-1,3,5(10)-trien-6-one, 3,16,17-trihydroxy-,
O-[(3,5-difluorophenyl)methyl]oxime, (16 α ,17 β)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.



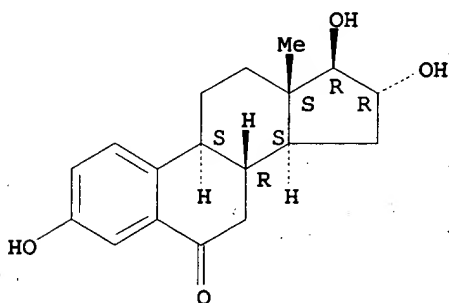
IT 7323-86-6

RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of estratriene derivs. for treating asthma and airway diseases)

RN 7323-86-6 HCAPLUS

CN Estradiol-1,3,5(10)-trien-6-one, 3,16,17-trihydroxy-,
(16 α ,17 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IC ICM C07J041-00

ICS C07J043-00; A61K031-565; A61P011-06; A61P029-00
32-3 (Steroids)

Section cross-reference(s): 1, 2, 63

IT Estrogen receptors

Tubulins

RL: BSU (Biological study, unclassified); BIOL (Biological study)
(preparation of estratriene derivs. and their affinity for the
estrogen receptor and tubulin)

IT Estrogens

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic
preparation); THU (Therapeutic use); BIOL (Biological study); PREP
(Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of estratriene derivs. for treating asthma and airway
diseases)

IT	94714-28-0P	796060-85-0P	796060-89-4P	796060-90-7P
	796060-91-8P	796847-95-5P	796847-96-6P	796847-97-7P
	796847-98-8P	796847-99-9P	796848-00-5P	796848-01-6P
	796848-02-7P	796848-03-8P	796848-04-9P	796848-05-0P
	796848-06-1P	796848-07-2P	796848-08-3P	796848-09-4P
	796848-10-7P	796848-11-8P	796848-12-9P	796848-13-0P

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796848-26-5P 796848-27-6P 796848-28-7P 796848-29-8P
 796848-30-1P 796848-31-2P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation);
THU (Therapeutic use); BIOL (Biological study); PREP
 (Preparation); USES (Uses)

(preparation of estratriene derivs. for treating asthma and airway diseases)

IT 104-81-4, 4-Methylbenzyl bromide 119-26-6, 2,4-Dinitrophenylhydrazine 362-07-2, 2-Methoxyestradiol 362-08-3, 2-Methoxyestrone 524-38-9, N-Hydroxyphthalimide 593-56-6, Methoxylamine hydrochloride 705-29-3, 3-Trifluoromethylbenzyl chloride 824-94-2, 4-Methoxybenzyl chloride 874-98-6, 3-Methoxybenzyl bromide 1944-96-3, O-(4-Nitrobenzyl)hydroxylamine 2086-26-2, O-(4-Nitrobenzyl)hydroxylamine hydrochloride 2687-43-6, O-Benzylhydroxylamine hydrochloride 3958-60-9, 2-Nitrobenzyl bromide 6599-97-9 **7323-86-6** 7647-01-0, Hydrochloric acid, reactions 7803-49-8, Hydroxylamine, reactions 17201-43-3, 4-Cyanobenzyl bromide 21101-63-3, 4-Trifluoromethylthiobenzyl bromide 28188-41-2, 3-Cyanobenzyl bromide 38002-18-5 50824-05-0, 4-Trifluoromethoxybenzyl bromide 52552-21-3 73789-86-3, 4-Isopropylbenzyl bromide 73870-24-3, (4-Bromomethyl)pyridine hydrobromide 141776-91-2, 3,5-Difluorobenzyl bromide 159689-88-0, 3-Trifluoromethoxybenzyl bromide 796061-03-5 796061-05-7

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of estratriene derivs. for treating asthma and airway diseases)

REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L53 ANSWER 4 OF 16 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:927229 HCAPLUS

DOCUMENT NUMBER: 141:395713

TITLE: Preparation of 8 β -vinyl-11 β -(ω -substituted)alkyl-estra-1,3,5(10)-trienes as ER β antagonists

INVENTOR(S): Braeuer, Nico; Peters, Olaf; Hillisch, Alexander; Bohlmann, Rolf; Richter, Margit; Muhn, Hans Peter

PATENT ASSIGNEE(S): Schering Aktiengesellschaft, Germany

SOURCE: PCT Int. Appl., 84 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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WO 2004094451	A2	20041104	WO 2004-EP4086	
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2004

0416

WO 2004094451	A3	20041223		
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W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW

RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW,
AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY,
CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC,
NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM,
GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

DE 10318896 A1 20041125 DE 2003-10318896

2003
0422

CA 2522354 AA 20041104 CA 2004-2522354

2004
0416

EP 1622924 A2 20060208 EP 2004-727876

2004
0416

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE,
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EE, HU, PL, SK, HR

US 2005065135 A1 20050324 US 2004-829390

2004
0422

PRIORITY APPLN. INFO.:

DE 2003-10318896 A

2003
0422

US 2003-464630P P

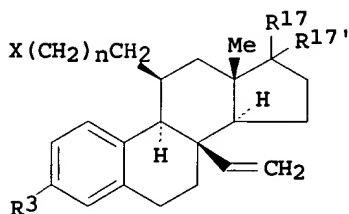
2003
0423

WO 2004-EP4086 W

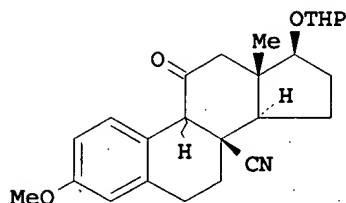
2004
0416

OTHER SOURCE(S):
GI

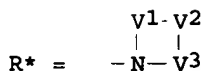
MARPAT 141:395713



I



II



AB The invention relates to 8 β -vinyl-11 β -(ω -substituted)alkyl-estra-1,3,5(10)-trienes I [R3 = OR19, OSO2R20, OC(:O)R21; n = 3, 4, 5; X = CWYZ; Z, W = R19; WZ = O (then Y = R19, R20); R17R17' = O, CR23R24 (with R23, R24 = H, halogen); R17 = H, OR19, halogen; R17' = R19, OSO2R20, C(:O)R21, OC(:O)R21; R19 = H, CpFqHr (p = 1 - 9; q > 1 and q + r = 2p + 1), unbranched C1-8-alkyl, branched C5-6-alkyl, Ph, C3-6-cycloalkyl, (C3-6-cycloalkyl)-(C1-4-alkylene), (un)branched C2-5-alkenyl, alkynyl, (un)substituted aryl, heteroaryl, heterocycle,

aryl-(C1-4-alkylene), heteroaryl-(C1-4-alkylene); R20 = NR21R22, CH:NOR19, R*; V1 = (CH2)m; V2 = CH2, O, S, NR25; V3 = (CH2)o; M = 0 - 8; o = 0 - 8; m + o = 2 - 12; R21, R22 = R19; R25 = R19, R20SO2, C(:O)R21], which have ER β antagonistic activity, methods for the production thereof, the intermediate products thereof, pharmaceutical preps. containing the inventive compds., and the use thereof for producing medicaments. Thus, I [R3 = OH, R17 = β -OH, R17' = α -H, X = CH(OH)CF3, n = 3] was prepared from estratrienone II in 10 steps. The novel compds. can be used for contraceptive purposes in men and women without influencing other estrogen-sensitive organs such as the uterus or the liver and while also being suitable for the treatment of benign or malignant proliferous ovarian diseases, such as ovarian carcinoma and granulosa cell tumors. The ER β antagonistic activity of I [R3 = OH, R17 = β -OH, R17' = α -H, X = CH(OH)CF3, n = 3] was determined [EC50 = 0.8 vs. ER α (at 0.38 nM) and EC50 = 42 vs. ER β (at 0.49 nM)].

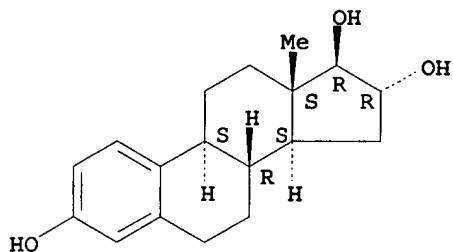
IT 50-27-1, Estriol

RL: PAC (Pharmacological activity); BIOL (Biological study)
(preparation of 8 β -vinyl-11 β -(ω -substituted)alkyl-estra-1,3,5(10)-trienes as ER β antagonists)

RN 50-27-1 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16,17-triol, (16 α ,17 β)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.



IC ICM C07J075-00

CC 32-3 (Steroids)

Section cross-reference(s): 1, 2, 63

ST estratriene alkyl vinyl deriv prepn **estrogen** receptor
beta antagonist; contraceptive male female estratriene alkyl vinyl
deriv prepn; malignant proliferous ovarian disease therapeutic
estratriene alkyl vinyl deriv; ovarian carcinoma therapeutic
estratriene alkyl vinyl deriv; granulosa cell tumor therapeutic
estratriene alkyl vinyl deriv

IT Liver

Uterus

(**estrogen**-sensitive organ, unaffected; preparation of
8 β -vinyl-11 β -(ω -substituted)alkyl-estra-
1,3,5(10)-trienes as ER β antagonists)

IT Antiestrogens

Estrogens

RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL
(Biological study); PREP (Preparation); USES (Uses)
(preparation of 8 β -vinyl-11 β -(ω -substituted)alkyl-
estra-1,3,5(10)-trienes as ER β antagonists)

IT **Estrogen** receptors

RL: BSU (Biological study, unclassified); BIOL (Biological study)
(α ; preparation of 8 β -vinyl-11 β -(ω -
substituted)alkyl-estra-1,3,5(10)-trienes as ER β
antagonists)

IT **Estrogen** receptors

RL: BSU (Biological study, unclassified); BIOL (Biological study)

(β , antagonists; preparation of 8 β -vinyl-11 β -(ω -substituted)alkyl-estra-1,3,5(10)-trienes as ER β antagonists)

IT 50-27-1, Estriol 53-16-7, Estrone, biological studies
57-91-0, 17 α -Estradiol 521-17-5, 5-Androstenediol
98008-06-1 367269-67-8 367269-80-5
RL: PAC (Pharmacological activity); BIOL (Biological study)
(preparation of 8 β -vinyl-11 β -(ω -substituted)alkyl-estra-1,3,5(10)-trienes as ER β antagonists)

L53 ANSWER 5 OF 16 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:412956 HCAPLUS

DOCUMENT NUMBER: 140:423862

TITLE: Process for preparation of estetrol from estrone derived steroids

INVENTOR(S): Verhaar, Mark Theodoor; Koch, Thomas; Warmerdan, Erwin Gerardus Jacobus

PATENT ASSIGNEE(S): Pantarhei Bioscience B.V., Neth.; Warmerdam, Erwin, Gerardus, Jacobus

SOURCE: PCT Int. Appl., 33 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

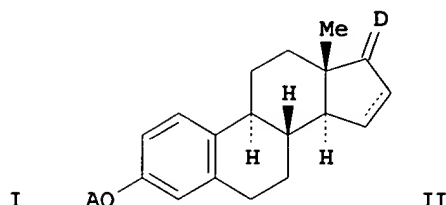
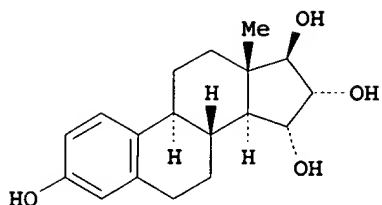
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004041839	A2	20040521	WO 2003-NL782	2003 1107
WO 2004041839	A3	20040701		
WO 2004041839	C1	20050721		
W:				
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RW:				
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CA 2505190	AA	20040521	CA 2003-2505190	2003 1107
AU 2003279624	A1	20040607	AU 2003-279624	2003 1107
EP 1562976	A2	20050817	EP 2003-772962	2003 1107
R:				
AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
CN 1735627	A	20060215	CN 2003-80108518	2003 1107
PRIORITY APPLN. INFO.:			EP 2002-79676	A 2002 1108
			WO 2003-NL782	W

2003
1107

OTHER SOURCE(S): CASREACT 140:423862; MARPAT 140:423862
GI



AB The present invention discloses a process for preparing estetrol (I) from estrone II (A = H, D = O, dashed bond = single bond) and estrone derived steroids, such as II [A = C1-C5 alkyl group, preferably a Me group, or a C7-C12 benzylic group, preferably a benzyl group; D = O, ethylene dioxy; dashed bond = single bond or double bond]. This process is particularly suitable to industry. The use of the prepared compds. for the manufacture of a pharmaceutical composition for hormone replacement therapy, treating or preventing a disorder from the group consisting of autoimmune diseases, breast tumors and colorectal tumors is also claimed.

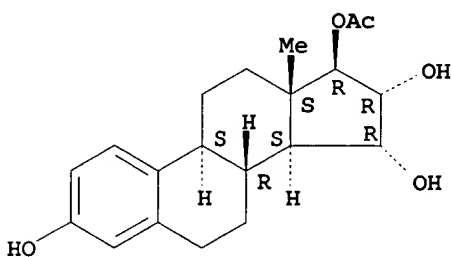
IT 690996-23-7P

RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of estetrol via estrone derived steroids)

RN 690996-23-7 HCAPLUS

CN Estrone-1,3,5(10)-triene-3,15,16,17-tetrol, 17-acetate, (15 α ,16 α ,17 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



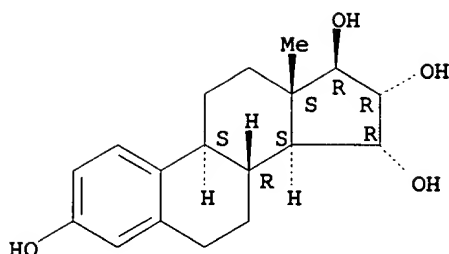
IT 15183-37-6P, Estetrol

RL: IMF (Industrial manufacture); SPN (Synthetic preparation);
PREP (Preparation)
(preparation of estetrol via estrone derived steroids)

RN 15183-37-6 HCAPLUS

CN Estrone-1,3,5(10)-triene-3,15,16,17-tetrol, (15 α ,16 α ,17 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IC ICM C07J001-00

CC 32-3 (Steroids)

Section cross-reference(s): 62, 63

IT Estrogens

RL: RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(preparation of estetrol via estrone derived steroids for the manufacture of a pharmaceutical composition for use for hormone replacement therapy, treating or preventing breast tumors and colorectal tumors and promoting wound healing)

IT 138743-03-0P 534572-67-3P 690996-23-7P 690996-24-8P
690996-25-9P 690996-26-0P 690996-27-1P

RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of estetrol via estrone derived steroids)

IT 15183-37-6P, Estetrol

RL: IMF (Industrial manufacture); SPN (Synthetic preparation);
PREP (Preparation)
(preparation of estetrol via estrone derived steroids)

L53 ANSWER 6 OF 16 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2003:991529 HCAPLUS

DOCUMENT NUMBER: 140:42342

TITLE: Preparation of 9 α -substituted
estratrienes as selectively active
estrogens

INVENTOR(S): Kosemund, Dirk; Mueller, Gerd; Hillisch,
Alexander; Fritzemeier, Karl-Heinrich; Muhn,
Peter

PATENT ASSIGNEE(S): Schering Aktiengesellschaft, Germany

SOURCE: PCT Int. Appl., 45 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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WO 2003104253	A2	20031218	WO 2003-EP6172	
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2003
0611

WO 2003104253	A3	20040916		
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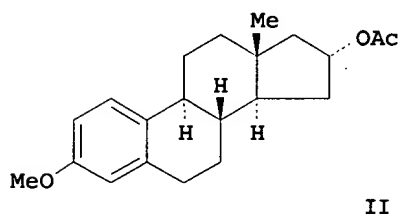
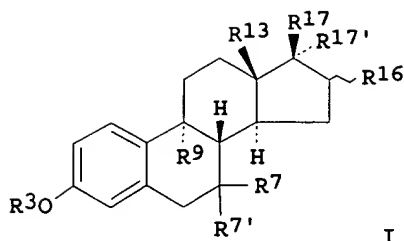
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CH, CN, CO, CR, CU, CZ, DK, DM, DZ, EC, EE, ES, FI, GB,
GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP,
KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN,
MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD,
SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC,
VN, YU, ZA, ZM, ZW

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM,

AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ,
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 PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN,
 GQ, GW, ML, MR, NE, SN, TD, TG

DE 10226326	A1	20040115	DE 2002-10226326	2002 0611
CA 2486495	AA	20031218	CA 2003-2486495	2003 0611
US 2004087565	A1	20040506	US 2003-458735	2003 0611
EP 1517914	A2	20050330	EP 2003-757065	2003 0611
EP 1517914	B1	20050831		
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BR 2003012140	A	20050405	BR 2003-12140	2003 0611
AT 303397	E	20050915	AT 2003-757065	2003 0611
JP 2005533053	T2	20051104	JP 2004-511321	2003 0611
NO 2005000127	A	20050311	NO 2005-127	2005 0110
PRIORITY APPLN. INFO.:			DE 2002-10226326	A 2002 0611
			US 2003-443868P	P 2003 0131
			WO 2003-EP6172	W 2003 0611

OTHER SOURCE(S): MARPAT 140:42342
 GI

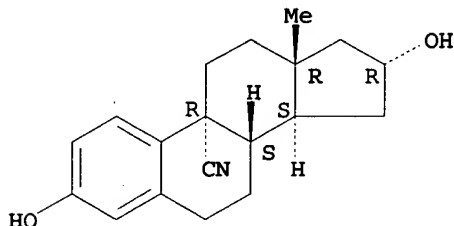


AB The invention relates to novel 9 α -substituted estratrienes I [R3 = H, R18; R7, R7' = H, halogen; R9 = (un)branched C2-6-alkenyl (optionally partially or fully halogenated), ethynyl, prop-1-ynyl; R13 = Me, Et; R16 = OH, OR18, ; R17, R17' = H, halogen; R18 = (un)branched, (un)saturated C1-6-hydrocarbon, CF3, (un)substituted aryl, heteroaryl, aralkyl, COR19; R19 = (un)branched, (un)saturated (up to three), C1-10-hydrocarbon (optionally substituted partially or fully with halogens); R20 = NR21R22, C1-5-alkyl, C(O)R23 ; R21, R22 = H, C1-5-alkyl, C(O)R23; R23 = (un)substituted, (un)branched, (un)saturated (up to three) C1-10-hydrocarbon (optionally substituted partially or fully with halogens), C3-7-cycloalkyl, (un)substituted C4-15-cycloalkylaryl, (un)substituted aryl; NR23 = C2-6-polymethyleneimino, morpholino] as pharmaceutical active ingredients which have, in vitro, a higher affinity to **estrogen** receptor preps. of the rat prostate than to **estrogen** receptor preparation of the rat uterus, and, in vivo, preferably a preferential action on the ovary compared to the uterus. The invention also relates to the production of said estratrienes, to the therapeutic application thereof and to pharmaceutical forms of administration containing the novel compds. Thus, 9 α -vinylestra-1,3,5(10)-triene-3,16 α -diol (I; R3 = R7 = R7' = R17 = R17' = H, R9 = CH:CH2, R13 = Me, R16 = α -OH) was prepared from 3-methoxyestra-1,3,5(10)-triene-16 α -yl acetate (II) via regioselective and stereoselective cyanation with TMSCN in CH2Cl2 containing LiClO4 and DDQ, O-demethylation with TMSCl/NaI in MeCN, deacetylation with K2CO3 in MeOH, reduction with Dibal-H in PhMe, and Wittig reaction with MePh3PI in DMSO containing NaH. The invention further relates to the use of said compds. for treating illnesses and states related to **estrogen** deficiency. The receptor binding activity of 9 α -vinylestra-1,3,5(10)-triene-3,16 α -diol (I; R3 = R7 = R7' = R17 = R17' = H, R9 = CH:CH2, R13 = Me, R16 = α -OH) was determined [RBA = 1.2 (for rat uterus); RBA = 100 (for rat prostate)].

IT 634910-63-7P, 3,16 α -Dihydroxyestra-1,3,5(10)-triene-9 α -carbonitrile
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and Dibal reduction of; preparation of 9 α -substituted estratrienes as selectively active **estrogens**)

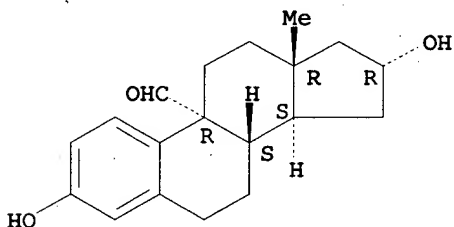
RN 634910-63-7 HCAPLUS
 CN Estr-1,3,5(10)-triene-9-carbonitrile, 3,16-dihydroxy-,
 (16 α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



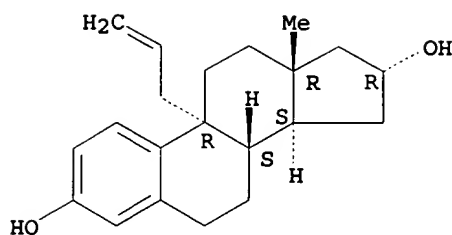
IT 634910-64-8P, 3,16 α -Dihydroxyestra-1,3,5(10)-triene-
 9 α -carboxaldehyde
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP
 (Preparation); RACT (Reactant or reagent)
 (preparation and Wittig reactions of; preparation of 9 α -substituted
 estratrienes as selectively active **estrogens**)
 RN 634910-64-8 HCAPLUS
 CN Estr-1,3,5(10)-triene-9-carboxaldehyde, 3,16-dihydroxy-,
 (16 α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 634891-19-3P 634891-20-6P 634891-39-7P
 634891-40-0P 634891-41-1P 634891-47-7P
 634891-48-8P 634891-49-9P 634891-50-2P
 634891-51-3P 634891-52-4P 634891-53-5P
 634910-53-5P, 9 α -Vinylestra-1,3,5(10)-triene-
 3,16 α -diol 634910-54-6P, 9 α -Vinyl-18 α -
 homoestra-1,3,5(10)-triene-3,16 α -diol 634910-55-7P
 , 9 α -(2,2-Difluorovinyl)estra-1,3,5(10)-triene-3,16 α -
 diol 634910-56-8P, 9 α -(2,2-Difluorovinyl)-18 α -
 homoestra-1,3,5(10)-triene-3,16 α -diol 634910-57-9P
 , 17 β -Fluoro-9 α -vinylestra-1,3,5(10)-triene-3,16 α -
 diol 634910-58-0P, 17,17-Difluoro-9 α -vinylestra-
 1,3,5(10)-triene-3,16 α -diol 634910-59-1P,
 9 α -(1-Hexenyl)estra-1,3,5(10)-triene-3,16 α -diol
 634910-60-4P, 9 α -(1-Butenyl)estra-1,3,5(10)-triene-
 3,16 α -diol
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation);
 THU (Therapeutic use); BIOL (Biological study); PREP
 (Preparation); USES (Uses)
 (preparation of 9 α -substituted estratrienes as selectively
 active **estrogens**)
 RN 634891-19-3 HCAPLUS
 CN Estr-1,3,5(10)-triene-3,16-diol, 9-(2-propenyl)-, (16 α)-
 (9CI) (CA INDEX NAME)

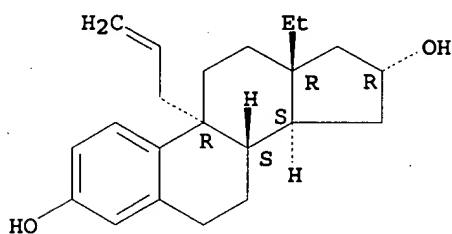
Absolute stereochemistry.



RN 634891-20-6 HCAPLUS

CN Gona-1,3,5(10)-triene-3,16-diol, 13-ethyl-9-(2-propenyl)-,
(16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

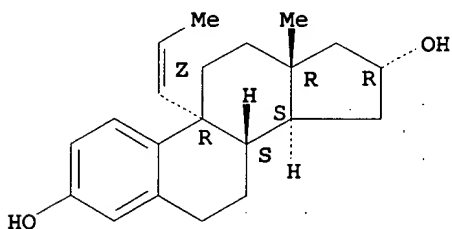


RN 634891-39-7 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 9-(1Z)-1-propenyl-, (16α)-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.

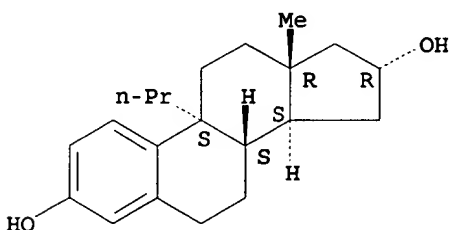
Double bond geometry as shown.



RN 634891-40-0 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 9-propyl-, (16α)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.

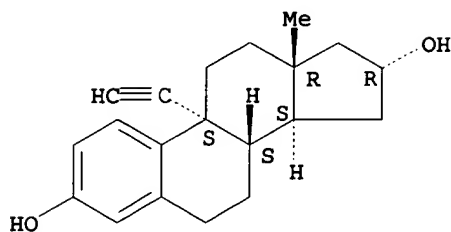


RN 634891-41-1 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 9-ethynyl-, (16α)- (9CI)

(CA INDEX NAME)

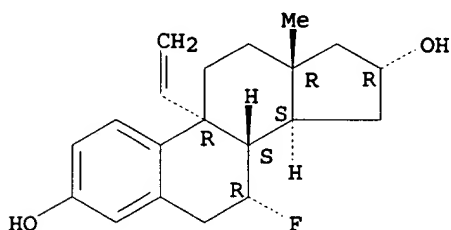
Absolute stereochemistry.



RN 634891-47-7 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 9-ethenyl-7-fluoro-,
(7 α ,16 α)- (9CI) (CA INDEX NAME)

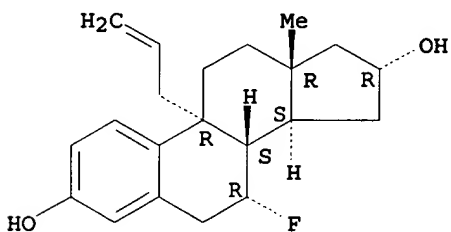
Absolute stereochemistry.



RN 634891-48-8 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 7-fluoro-9-(2-propenyl)-,
(7 α ,16 α)- (9CI) (CA INDEX NAME)

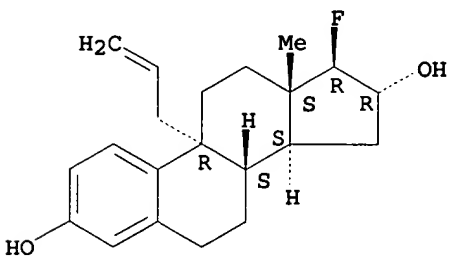
Absolute stereochemistry.



RN 634891-49-9 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 17-fluoro-9-(2-propenyl)-,
(16 α ,17 β)- (9CI) (CA INDEX NAME)

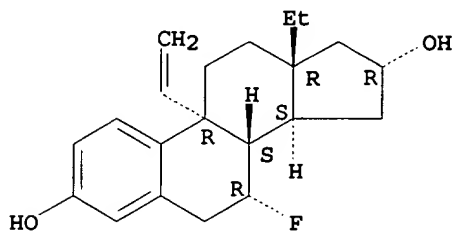
Absolute stereochemistry.



RN 634891-50-2 HCAPLUS

CN Gona-1,3,5(10)-triene-3,16-diol, 9-ethenyl-13-ethyl-7-fluoro-,
(7 α ,16 α)- (9CI) (CA INDEX NAME)

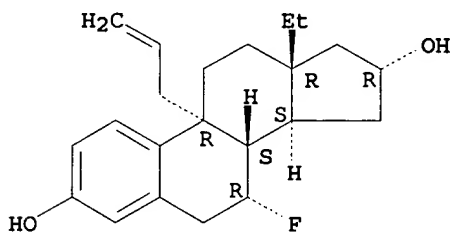
Absolute stereochemistry.



RN 634891-51-3 HCAPLUS

CN Gona-1,3,5(10)-triene-3,16-diol, 13-ethyl-7-fluoro-9-(2-propenyl)-
, (7 α ,16 α)- (9CI) (CA INDEX NAME)

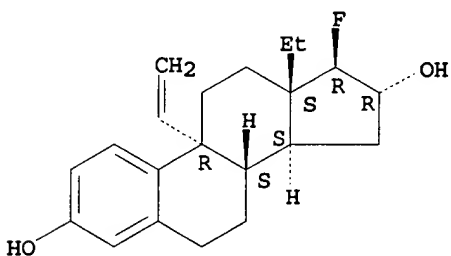
Absolute stereochemistry.



RN 634891-52-4 HCAPLUS

CN Gona-1,3,5(10)-triene-3,16-diol, 9-ethenyl-13-ethyl-17-fluoro-,
(16 α ,17 β)- (9CI) (CA INDEX NAME)

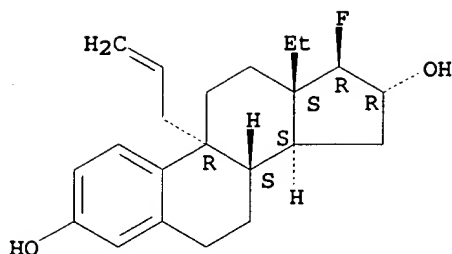
Absolute stereochemistry.



RN 634891-53-5 HCAPLUS

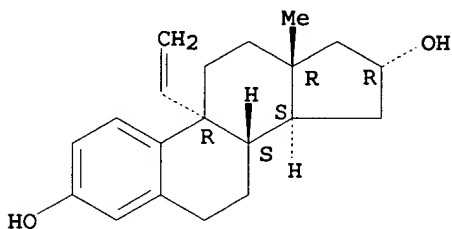
CN Gona-1,3,5(10)-triene-3,16-diol, 13-ethyl-17-fluoro-9-(2-propenyl)-
, (16 α ,17 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



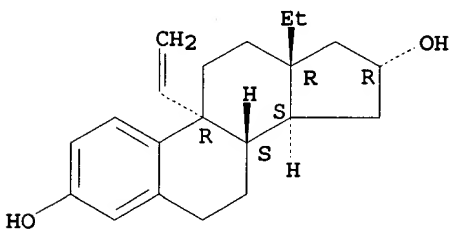
RN 634910-53-5 HCAPLUS
 CN Estra-1,3,5(10)-triene-3,16-diol, 9-ethenyl-, (16α)- (9CI)
 (CA INDEX NAME)

Absolute stereochemistry.



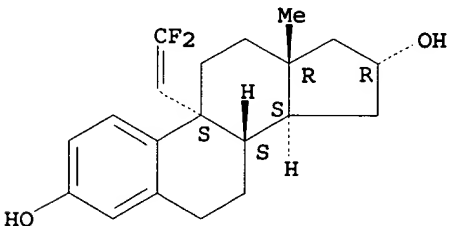
RN 634910-54-6 HCAPLUS
 CN Gona-1,3,5(10)-triene-3,16-diol, 9-ethenyl-13-ethyl-, (16α)-
 (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 634910-55-7 HCAPLUS
 CN Estra-1,3,5(10)-triene-3,16-diol, 9-(2,2-difluoroethenyl)-,
 (16α)- (9CI) (CA INDEX NAME)

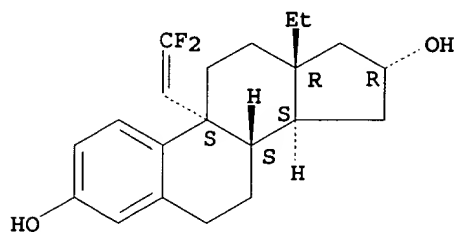
Absolute stereochemistry.



RN 634910-56-8 HCAPLUS
 CN Gona-1,3,5(10)-triene-3,16-diol, 9-(2,2-difluoroethenyl)-13-ethyl-

, (16 α)- (9CI) (CA INDEX NAME)

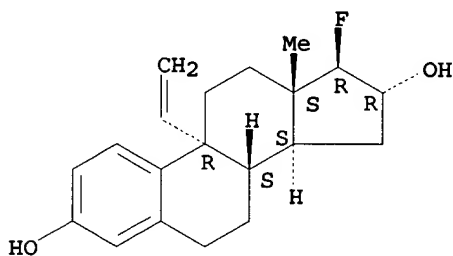
Absolute stereochemistry.



RN 634910-57-9 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 9-ethenyl-17-fluoro-,
(16 α ,17 β)- (9CI) (CA INDEX NAME)

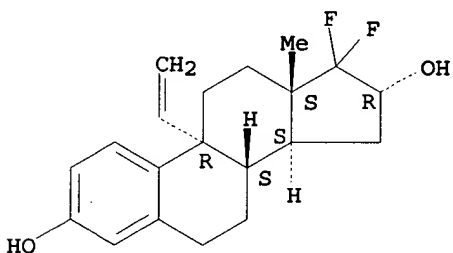
Absolute stereochemistry.



RN 634910-58-0 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 9-ethenyl-17,17-difluoro-,
(16 α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

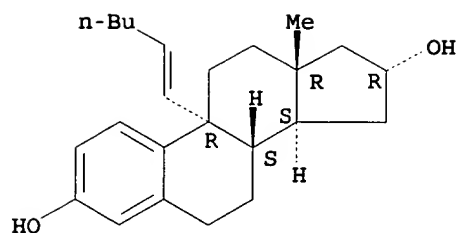


RN 634910-59-1 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 9-(1-hexenyl)-, (16 α)-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.

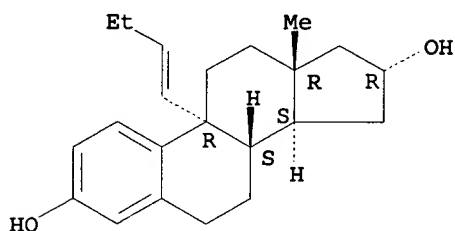


RN 634910-60-4 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 9-(1-butenyl)-, (16α)-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.



IT 50-27-1, Estriol

RL: PAC (Pharmacological activity); THU (Therapeutic use)

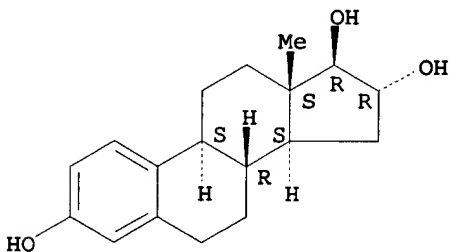
; BIOL (Biological study); USES (Uses)

(preparation of 9α-substituted estratrienes as selectively
active **estrogens**)

RN 50-27-1 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16,17-triol, (16α,17β)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.



IC ICM C07J

CC 32-3 (**Steroids**)

Section cross-reference(s): 1, 2, 63

ST estratriene steroid prepn **estrogenic** activity
estrogen receptor binding

IT Steroids, preparation

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic
preparation); THU (Therapeutic use); BIOL (Biological study); PREP
(Preparation); RACT (Reactant or reagent); USES (Uses)

(9α-substituted estratrienes; preparation of

9α-substituted estratrienes as selectively active
estrogens)

IT Prostate gland, disease

- (benign hyperplasia, medicaments; preparation of 9 α -substituted estratrienes as selectively active **estrogens**)
- IT Hyperplasia
(benign prostatic, medicaments; preparation of 9 α -substituted estratrienes as selectively active **estrogens**)
- IT **Estrogens**
(deficiency, diseases, medicaments; preparation of 9 α -substituted estratrienes as selectively active **estrogens**)
- IT Hormones, animal, biological studies
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(deficiency, medicaments; preparation of 9 α -substituted estratrienes as selectively active **estrogens**)
- IT Circulation
Immunity
(disorder, medicaments; preparation of 9 α -substituted estratrienes as selectively active **estrogens**)
- IT Fertility disorders
(female, medicaments; preparation of 9 α -substituted estratrienes as selectively active **estrogens**)
- IT Bone, disease
(mass loss, medicaments; preparation of 9 α -substituted estratrienes as selectively active **estrogens**)
- IT Autoimmune disease
Hormone replacement therapy
Multiple sclerosis
Osteoporosis
Ovary, disease
Rheumatoid arthritis
(medicaments; preparation of 9 α -substituted estratrienes as selectively active **estrogens**)
- IT **Estrogen receptors**
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(modulator synergism; preparation of 9 α -substituted estratrienes as selectively active **estrogens**)
- IT Pain
(ovarial, medicaments; preparation of 9 α -substituted estratrienes as selectively active **estrogens**)
- IT Analgesics
(ovary dysfunction (pain); preparation of 9 α -substituted estratrienes as selectively active **estrogens**)
- IT Menopause
(perimenopause, medicaments; preparation of 9 α -substituted estratrienes as selectively active **estrogens**)
- IT Menopause
(postmenopause, medicaments; preparation of 9 α -substituted estratrienes as selectively active **estrogens**)
- IT Antiarthritics
Antirheumatic agents
Bone resorption inhibitors
Cardiovascular agents
Human
(preparation of 9 α -substituted estratrienes as selectively active **estrogens**)
- IT Antiestrogens
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 9 α -substituted estratrienes as selectively active **estrogens**)
- IT 1478-53-1, Diethyl (difluoromethyl)phosphonate
RL: RCT (Reactant); RACT (Reactant or reagent)
(Horner-Emmons reaction of, with dihydroxyestratrienecarboxaldehyde; preparation of 9 α -substituted estratrienes as selectively active **estrogens**)

- IT 6228-47-3, Propyltriphenylphosphonium bromide 35171-55-2, Pentyltriphenylphosphonium iodide
RL: RCT (Reactant); RACT (Reactant or reagent)
(Wittig reaction of, with dihydroxyestratrienecarboxaldehyde; preparation of 9 α -substituted estratrienes as selectively active **estrogens**)
- IT 84449-90-1
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(**estrogen** receptor modulator co-drug; preparation of 9 α -substituted estratrienes as selectively active **estrogens**)
- IT 634910-63-7P, 3,16 α -Dihydroxyestra-1,3,5(10)-triene-9 α -carbonitrile 634910-66-0P, 3,16 α -Bis[(perhydropyran-2-yl)oxy]-18a-homoestra-1,3,5(10)-triene-9 α -carbonitrile 634910-68-2P, 3,16 α -Bis[(perhydropyran-2-yl)oxy]estra-1,3,5(10)-triene-9 α -carbonitrile 634910-71-7P, 3,16 α -Bis[(perhydropyran-2-yl)oxy]-17 β -fluoroestra-1,3,5(10)-triene-9 α -carbonitrile 634910-77-3P, 3,16 α -Bis[(perhydropyran-2-yl)oxy]-17,17-difluoroestra-1,3,5(10)-triene
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and Dibal reduction of; preparation of 9 α -substituted estratrienes as selectively active **estrogens**)
- IT 634910-61-5P, 9 α -Cyano-3-methoxyestra-1,3,5(10)-trien-16 α -yl acetate
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and O-demethylation of; preparation of 9 α -substituted estratrienes as selectively active **estrogens**)
- IT 634910-64-8P, 3,16 α -Dihydroxyestra-1,3,5(10)-triene-9 α -carboxaldehyde 634910-67-1P, 3,16 α -Dihydroxy-18a-homoestra-1,3,5(10)-triene-9 α -carboxaldehyde 634910-69-3P 634910-72-8P, 3,16 α -Dihydroxy-17 β -fluoroestra-1,3,5(10)-triene-9 α -carboxaldehyde 634910-74-0P, 3,16 α -Bis[(perhydropyran-2-yl)oxy]-17,17-difluoroestra-1,3,5(10)-triene-9 α -carboxaldehyde
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and Wittig reactions of; preparation of 9 α -substituted estratrienes as selectively active **estrogens**)
- IT 634910-62-6P, 9 α -Cyano-3-hydroxyestra-1,3,5(10)-trien-16 α -yl acetate
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and deacetylation of; preparation of 9 α -substituted estratrienes as selectively active **estrogens**)
- IT 634891-19-3P 634891-20-6P 634891-21-7P
634891-22-8P 634891-23-9P 634891-25-1P 634891-26-2P
634891-27-3P 634891-28-4P 634891-29-5P 634891-30-8P
634891-31-9P 634891-32-0P 634891-33-1P 634891-34-2P
634891-35-3P 634891-36-4P 634891-37-5P 634891-38-6P
634891-39-7P 634891-40-0P 634891-41-1P
634891-42-2P 634891-43-3P 634891-44-4P 634891-45-5P
634891-46-6P 634891-47-7P 634891-48-8P
634891-49-9P 634891-50-2P 634891-51-3P
634891-52-4P 634891-53-5P 634910-53-5P
, 9 α -Vinylestra-1,3,5(10)-triene-3,16 α -diol
634910-54-6P, 9 α -Vinyl-18a-homoestra-1,3,5(10)-triene-3,16 α -diol 634910-55-7P,
9 α -(2,2-Difluorovinyl)estra-1,3,5(10)-triene-3,16 α -diol 634910-56-8P, 9 α -(2,2-Difluorovinyl)-18a-homoestra-1,3,5(10)-triene-3,16 α -diol 634910-57-9P
, 17 β -Fluoro-9 α -vinylestra-1,3,5(10)-triene-3,16 α -diol 634910-58-0P, 17,17-Difluoro-9 α -vinylestra-

1,3,5(10)-triene-3,16 α -diol 634910-59-1P,
 9 α -(1-Hexenyl)estra-1,3,5(10)-triene-3,16 α -diol
 634910-60-4P, 9 α -(1-Butenyl)estra-1,3,5(10)-triene-
 3,16 α -diol

RL: PAC (Pharmacological activity); SPN (Synthetic preparation);
 THU (Therapeutic use); BIOL (Biological study); PREP
 (Preparation); USES (Uses)

(preparation of 9 α -substituted estratrienes as selectively
 active estrogens)

IT 50-27-1, Estriol 50-28-2, Estradiol, biological studies
 53-16-7, Estrone, biological studies 57-91-0,
 17 α -Estradiol 446-72-0, Genistein 479-13-0, Coumestrol
 521-17-5, 5-Androstenediol

RL: PAC (Pharmacological activity); THU (Therapeutic use)
 ; BIOL (Biological study); USES (Uses)

(preparation of 9 α -substituted estratrienes as selectively
 active estrogens)

IT 76820-87-6, 3-Methoxyestra-1,3,5(10)-trien-16 α -yl acetate
 634910-65-9, 3,16 α -Bis[(perhydropyran-2-yl)oxy]-18 α -
 homoestra-1,3,5(10)-triene 634910-70-6, 3,16 α -
 Bis[(perhydropyran-2-yl)oxy]-17 β -fluoroestra-1,3,5(10)-triene
 634910-73-9, 3,16 α -Bis[(perhydropyran-2-yl)oxy]-17,17-
 difluoroestra-1,3,5(10)-triene-9 α -carbonitrile
 634910-75-1, 3,16 α -Bis[(perhydropyran-2-yl)oxy]estra-
 1,3,5(10)-triene

RL: RCT (Reactant); RACT (Reactant or reagent)

(regioselective and stereoselective cyanation of; preparation of
 9 α -substituted estratrienes as selectively active
 estrogens)

L53 ANSWER 7 OF 16 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2003:777821 HCAPLUS

DOCUMENT NUMBER: 139:292396

TITLE: Preparation and anti-estrogen effect
 of 19-nor-17 α -pregna-1,3,5(10)-trien-
 17 β -ols with a 21,16 α -lactone ring
 substituted with a long chain at the 11 β
 position

INVENTOR(S): Mueller, Gerd; Hillisch, Alexander; Hoffmann,
 Jens; Fritzemeier, Karl-Heinrich

PATENT ASSIGNEE(S): Schering Aktiengesellschaft; Germany

SOURCE: PCT Int. Appl., 27 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 2

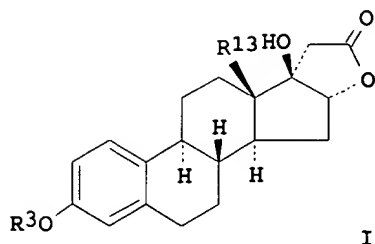
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003080641	A1	20031002	WO 2003-EP3226	2003 0327

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA,
 CH, CN, CO, CR, CU, CZ, DK, DM, DZ, EC, EE, ES, FI, GB,
 GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP,
 KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN,
 MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD,
 SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC,
 VN, YU, ZA, ZM, ZW
 RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
 AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ,
 DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL,
 PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN,
 GQ, GW, ML, MR, NE, SN, TD, TG

DE 10214180	A1	20031016	DE 2002-10214180	2002 0327
AU 2003221528	A1	20031008	AU 2003-221528	2003 0327
US 2003229059	A1	20031211	US 2003-397854	2003 0327
US 2004014735	A1	20040122	US 2003-397855	2003 0327
US 6956031	B2	20051018		
EP 1490391	A1	20041229	EP 2003-717244	2003 0327
EP 1490391	B1	20051221		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
JP 2005526805	T2	20050908	JP 2003-578394	2003 0327
AT 313552	E	20060115	AT 2003-717244	2003 0327
PRIORITY APPLN. INFO.:			DE 2002-10214180	A 2002 0327
			US 2002-374516P	P 2002 0423
			US 2002-374517P	P 2002 0423
			DE 2002-10214179	A 2002 0327
			WO 2003-EP3226	W 2003 0327

OTHER SOURCE(S): MARPAT 139:292396
GI



AB The invention relates to novel 19-nor-17 α -pregna-1,3,5(10)-trien-17 β -ols with a 21,16 α -lactone ring and a long chain substituent in the 11 β position, e.g., I [R3 =

C1-4-alkyl, C2-6-acyl, ; R11 = straight chain C6-17 alkyl group; R13 = Me, Et; R18 = NR19R20; R19, R20 = H, C1-5-alkyl, C(:O)R21; R21 =]. Thus, I [R3 = H, R11 = hexyl, R13 = Me] was prepared from 11 β -hexyl-17-oxoestra-1,3,5(10)-triene-3,16 α -diyl diacetate via condensation with acetonitrile lithium salt. The compds. have a tissue-selective pure anti-estrogen effect and are thus suitable for the production of medicaments. The estrogen receptor binding activity of was determined [RBA = 26.2 vs. rat uterus; RBA = 1.2 vs. rat prostate]; inhibition of MCF-7 mammary carcinoma cells by I [R3 = H, R11 = hexyl, R13 = Me] (at 1x10⁻⁵ M) was also determined

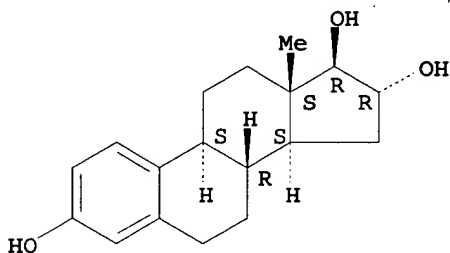
IT 50-27-1, Estriol

RL: PAC (Pharmacological activity); BIOL (Biological study)
(estrogen receptor binding activity of; preparation and anti-estrogen effect of 19-nor-17 α -pregna-1,3,5(10)-trien-17 β -ols 11 β -alkyl 21,16 α -lactone ring derivs.)

RN 50-27-1 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16,17-triol, (16 α ,17 β)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.



IC ICM C07J001-00

ICS A61K031-585; A61P035-00

CC 32-5 (Steroids)

Section cross-reference(s): 1, 2, 63

ST pregnane nor sterol lactone deriv antiestrogen antitumor;
norpregnatrienediol lactone prepn estrogen receptor
binding antiproliferative activity

IT Estrogen receptors

RL: BSU (Biological study, unclassified); BIOL (Biological study)
(binding activity; preparation and anti-estrogen effect of
19-nor-17 α -pregna-1,3,5(10)-trien-17 β -ols
11 β -alkyl 21,16 α -lactone ring derivs.)

IT Mammary gland, neoplasm

Prostate gland, neoplasm
(carcinoma, medicaments; preparation and anti-estrogen
effect of 19-nor-17 α -pregna-1,3,5(10)-trien-17 β -ols
11 β -alkyl 21,16 α -lactone ring derivs.)

IT Carcinoma

(endometrial, medicaments; preparation and anti-estrogen
effect of 19-nor-17 α -pregna-1,3,5(10)-trien-17 β -ols
11 β -alkyl 21,16 α -lactone ring derivs.)

IT Uterus, neoplasm

(endometrium, carcinoma, medicaments; preparation and anti-
estrogen effect of 19-nor-17 α -pregna-1,3,5(10)-
trien-17 β -ols 11 β -alkyl 21,16 α -lactone ring
derivs.)

IT Carcinoma

(mammary, medicaments; preparation and anti-estrogen
effect of 19-nor-17 α -pregna-1,3,5(10)-trien-17 β -ols
11 β -alkyl 21,16 α -lactone ring derivs.)

IT Sterols

RL: PAC (Pharmacological activity); SPN (Synthetic preparation);
THU (Therapeutic use); BIOL (Biological study); PREP
(Preparation); USES (Uses)

(norsterols; preparation and anti-estrogen effect of
19-nor-17 α -pregna-1,3,5(10)-trien-17 β -ols
11 β -alkyl 21,16 α -lactone ring derivs.)

IT Antitumor agents

Human

(preparation and anti-estrogen effect of
19-nor-17 α -pregna-1,3,5(10)-trien-17 β -ols
11 β -alkyl 21,16 α -lactone ring derivs.)

IT Antiestrogens

RL: PAC (Pharmacological activity); SPN (Synthetic preparation);
THU (Therapeutic use); BIOL (Biological study); PREP
(Preparation); USES (Uses)

(preparation and anti-estrogen effect of
19-nor-17 α -pregna-1,3,5(10)-trien-17 β -ols
11 β -alkyl 21,16 α -lactone ring derivs.)

IT Carcinoma

(prostatic, medicaments; preparation and anti-estrogen
effect of 19-nor-17 α -pregna-1,3,5(10)-trien-17 β -ols
11 β -alkyl 21,16 α -lactone ring derivs.)

IT 608101-30-0, 11 β -Hexyl-17-oxoestra-1,3,5(10)-triene-

3,16 α -diyl diacetate 608101-31-1, 11 β -Octyl-17-
oxoestra-1,3,5(10)-triene-3,16 α -diyl diacetate
608101-32-2, 11 β -Decyl-17-oxoestra-1,3,5(10)-triene-
3,16 α -diyl diacetate 608101-33-3, 11 β -Dodecyl-17-
oxoestra-1,3,5(10)-triene-3,16 α -diyl diacetate

RL: RCT (Reactant); RACT (Reactant or reagent)

(condensation with acetonitrile lithium salt; preparation and anti-
estrogen effect of 19-nor-17 α -pregna-1,3,5(10)-
trien-17 β -ols 11 β -alkyl 21,16 α -lactone ring
derivs.)

IT 50-27-1, Estriol 50-28-2, Estradiol, biological studies
53-16-7, Estrone, biological studies 57-91-0,
17 α -Estradiol 446-72-0, Genistein 479-13-0, Coumestrol
521-17-5, 5-Androstenediol

RL: PAC (Pharmacological activity); BIOL (Biological study)

(estrogen receptor binding activity of; preparation and
anti-estrogen effect of 19-nor-17 α -pregna-
1,3,5(10)-trien-17 β -ols 11 β -alkyl
21,16 α -lactone ring derivs.)

IT 608101-26-4P, 3,17 β -Dihydroxy-11 β -hexyl-19-nor-17 α -
pregna-1,3,5(10)-triene-21,16 α -lactone 608101-27-5P,

3,17 β -Dihydroxy-11 β -octyl-19-nor-17 α -pregna-
1,3,5(10)-triene-21,16 α -lactone 608101-28-6P,

3,17 β -Dihydroxy-11 β -decyl-19-nor-17 α -pregna-
1,3,5(10)-triene-21,16 α -lactone 608101-29-7P,

3,17 β -Dihydroxy-11 β -dodecyl-19-nor-17 α -pregna-
1,3,5(10)-triene-21,16 α -lactone

RL: PAC (Pharmacological activity); SPN (Synthetic preparation);

THU (Therapeutic use); BIOL (Biological study); PREP

(Preparation); USES (Uses)

(preparation and estrogen receptor binding activity of;
preparation and anti-estrogen effect of
19-nor-17 α -pregna-1,3,5(10)-trien-17 β -ols
11 β -alkyl 21,16 α -lactone ring derivs.)

REFERENCE COUNT:

6

THERE ARE 6 CITED REFERENCES AVAILABLE
FOR THIS RECORD. ALL CITATIONS AVAILABLE
IN THE RE FORMAT

L53 ANSWER 8 OF 16 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2003:331993 HCAPLUS

DOCUMENT NUMBER: 138:354135

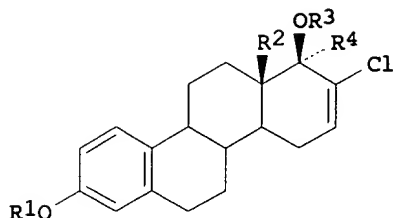
TITLE: Preparation of 17-chloro-D-homosteroid as
selective estrogen receptor

antagonists
 INVENTOR(S): Tornus, Ingo; Ring, Sven; Schubert, Gerd
 PATENT ASSIGNEE(S): Schering AG, Germany
 SOURCE: Ger. Offen., 12 pp.
 CODEN: GWXXBX
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 2
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 10151365	A1	20030430	DE 2001-10151365	2001 1017
WO 2002068548	A1	20020906	WO 2002-EP2117	2002 0227
WO 2002068548	C2	20030220		
WO 2002068548	A3	20030605		
WO 2002068548	C1	20031224		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2003083377	A1	20030501	US 2002-83685	2002 0227
US 6794409	B2	20040921		
EP 1365768	A2	20031203	EP 2002-706750	2002 0227
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2004529107	T2	20040924	JP 2002-568649	2002 0227
US 2005020695	A1	20050127	US 2004-909540	2004 0803
PRIORITY APPLN. INFO.:			US 2001-271409P	P 2001 0227
			DE 2001-10151365	A 2001 1017
			US 2001-329736P	P 2001 1018
			US 2002-83685	A3 2002 0227
			WO 2002-EP2117	W 2002

0227

OTHER SOURCE(S): CASREACT 138:354135; MARPAT 138:354135
GI



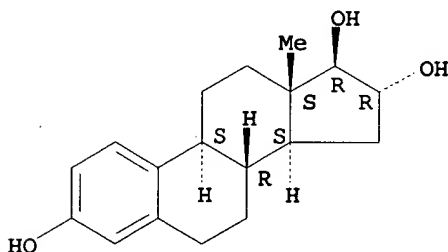
AB The present invention discloses preparation of 17-chloro-D-homosteroids, e.g., I [R1 = H, C1-6-alkanoyl, COPh; R2 = C1-6-alkyl; R3 = H, C1-6-alkyl, C1-6-alkanoyl, COPh; R4 = H, C1-6-alkyl, fluoroalkyl, C.tplbond.CR5; R5 = H, C1-6-alkyl, (un)substituted phenyl], for their use as selective **estrogen** receptor antagonists. Thus, I [R1 = R3 = H, R2 = Et, R4 = CH2C.tplbond.CH] was prepared from 3-methoxy-18a-homoestra-1,3,5(10)-trien-17 β -ol via Jones oxidation, enol silylation, ring expansion with sodium trichloroacetate. The new compds. are suitable for contraception with men and women, without affecting other **estrogenic**-sensitive organs like the uterus or the liver. They are also suitable for the treatment of benign or malignant proliferative illnesses of the ovaries, like ovarian carcinomas and Granulosa cell tumors.

IT 50-27-1, Estriol
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(preparation of 17-chloro-D-homosteroids as selective **estrogen** receptor antagonists)

RN 50-27-1 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16,17-triol, (16 α ,17 β)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.



IC ICM C07J063-00
ICS A61K031-565

CC 32-3 (Steroids)
Section cross-reference(s): 1, 2, 63

ST homosteroid chloro prepn **estrogen** receptor antagonist;
ovary proliferative illness treatment chlorohomosteroid; ovarian carcinoma treatment chlorohomosteroid; Granulosa cell tumor treatment chlorohomosteroid

IT Coupling reaction
(Sonagashira; preparation of 17-chloro-D-homosteroids as selective **estrogen** receptor antagonists)

- IT Progesterone receptors
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(antagonist; preparation of 17-chloro-D-homosteroids as selective
estrogen receptor antagonists)
- IT **Estrogen** receptors
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(antagonists; preparation of 17-chloro-D-homosteroids as selective
estrogen receptor antagonists)
- IT Ovulation
(control; preparation of 17-chloro-D-homosteroids as selective
estrogen receptor antagonists)
- IT Contraceptives
(female; preparation of 17-chloro-D-homosteroids as selective
estrogen receptor antagonists)
- IT Ovary
(follicle cell, early genesis, promotion; preparation of
17-chloro-D-homosteroids as selective **estrogen**
receptor antagonists)
- IT Ovary, neoplasm
(granulosa cell, treatment; preparation of 17-chloro-D-homosteroids
as selective **estrogen** receptor antagonists)
- IT Contraceptives
(male; preparation of 17-chloro-D-homosteroids as selective
estrogen receptor antagonists)
- IT Progestogens
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(mesoproggestins; preparation of 17-chloro-D-homosteroids as
selective **estrogen** receptor antagonists)
- IT Organometallic compounds
RL: RGT (Reagent); RACT (Reactant or reagent)
(organolithium reaction with acetylene or its alkyl or aryl
derivs.; preparation of 17-chloro-D-homosteroids as selective
estrogen receptor antagonists)
- IT Silanes
RL: RCT (Reactant); RACT (Reactant or reagent)
(organosilanes, with 17-chloro-D-homoestrone; preparation of
17-chloro-D-homosteroids as selective **estrogen**
receptor antagonists)
- IT Human
(preparation of 17-chloro-D-homosteroids as selective
estrogen receptor antagonists)
- IT **Estrogens**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation);
THU (Therapeutic use); BIOL (Biological study); PREP
(Preparation); USES (Uses)
(preparation of 17-chloro-D-homosteroids as selective
estrogen receptor antagonists)
- IT Ovary, disease
(proliferative, treatment; preparation of 17-chloro-D-homosteroids
as selective **estrogen** receptor antagonists)
- IT Grignard reagents
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with 17-chloro-D-homoestrone; preparation of
17-chloro-D-homosteroids as selective **estrogen**
receptor antagonists)
- IT Ovary, neoplasm
(treatment; preparation of 17-chloro-D-homosteroids as selective
estrogen receptor antagonists)
- IT 3625-82-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(Jones oxidation of; preparation of 17-chloro-D-homosteroids as
selective **estrogen** receptor antagonists)
- IT 454485-63-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(O-demethylation of; preparation of 17-chloro-D-homosteroids as
selective **estrogen** receptor antagonists)

- IT 9034-40-6, GnRH
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(antagonists; preparation of 17-chloro-D-homosteroids as selective
estrogen receptor antagonists)
- IT 865-47-4
RL: RGT (Reagent); RACT (Reactant or reagent)
(deprotonation by, of acetylene in reaction with
17-chloro-D-homoestrone; preparation of 17-chloro-D-homosteroids as
selective **estrogen** receptor antagonists)
- IT 1624-62-0, 3-Methoxyestra-1,3,5(10)-trien-17-one
RL: RCT (Reactant); RACT (Reactant or reagent)
(enol silylation of; preparation of 17-chloro-D-homosteroids as
selective **estrogen** receptor antagonists)
- IT 454485-57-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation and O-demethylation of; preparation of 17-chloro-D-
homosteroids as selective **estrogen** receptor
antagonists)
- IT 454485-55-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and O-demethylation of; preparation of 17-chloro-D-
homosteroids as selective **estrogen** receptor
antagonists)
- IT 454485-60-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and desilylation of; preparation of 17-chloro-D-homosteroids
as selective **estrogen** receptor antagonists)
- IT 848-04-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and enol silylation of; preparation of 17-chloro-D-
homosteroids as selective **estrogen** receptor
antagonists)
- IT 454485-56-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP
(Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with alkynylmagnesium bromides; preparation
of 17-chloro-D-homosteroids as selective **estrogen**
receptor antagonists)
- IT 454485-58-6P, 17-Chloro-3-methoxy-17a-homoestra-1,3,5(10),16-
tetraen-17a-one
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and reaction of, with methylmagnesium bromide or
(trifluoromethyl)trimethylsilane; preparation of
17-chloro-D-homosteroids as selective **estrogen**
receptor antagonists)
- IT 454485-61-1P 454485-62-2P 454485-64-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and reductive demethylation of; preparation of
17-chloro-D-homosteroids as selective **estrogen**
receptor antagonists)
- IT 115419-13-1P, 3-Methoxy-17-[(trimethylsilyl)oxy]estra-1,3,5(10)-
triene 518045-87-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP
(Preparation); RACT (Reactant or reagent)
(preparation and ring expansion of, with sodium trichloroacetate;
preparation of 17-chloro-D-homosteroids as selective
estrogen receptor antagonists)
- IT 454485-33-7P 454485-34-8P 454485-36-0P 454485-37-1P
454485-38-2P 454485-39-3P 454485-40-6P 454485-41-7P
454485-42-8P 454485-43-9P 454485-44-0P 454485-45-1P
454485-46-2P 454485-47-3P 454485-48-4P 454485-49-5P
454485-52-0P 454485-53-1P 454485-54-2P 518045-83-5P
518045-85-7P 518045-86-8P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation);
THU (Therapeutic use); BIOL (Biological study); PREP
(Preparation); USES (Uses)

- (preparation of 17-chloro-D-homosteroids as selective
estrogen receptor antagonists)
- IT 50-27-1, Estriol 50-28-2, Estradiol, biological studies
53-16-7, Estrone, biological studies 57-91-0,
17 α -Estradiol 446-72-0, Genistein 479-13-0, Coumestrol
521-17-5, 5-Androstene-diol
RL: PAC (Pharmacological activity); THU (Therapeutic use)
; BIOL (Biological study); USES (Uses)
- (preparation of 17-chloro-D-homosteroids as selective
estrogen receptor antagonists)
- IT 354-64-3, Pentafluoroethyl iodide 3466-32-8, 4-
Bromophenylmethylsulfone 4301-14-8, Ethynylmagnesium bromide
16466-97-0, (1-Propynyl)magnesium bromide
RL: RCT (Reactant); RACT (Reactant or reagent)
- (preparation of 17-chloro-D-homosteroids as selective
estrogen receptor antagonists)
- IT 74-86-2, Acetylene, reactions 81290-20-2,
(Trifluoromethyl)trimethylsilane
RL: RCT (Reactant); RACT (Reactant or reagent)
- (reaction of, with 17-chloro-D-homoestrone; preparation of
17-chloro-D-homosteroids as selective **estrogen**
receptor antagonists)
- IT 91935-83-0, Pentafluoroethyl lithium
RL: RGT (Reagent); RACT (Reactant or reagent)
- (reaction of, with 17-chloro-D-homoestrone; preparation of
17-chloro-D-homosteroids as selective **estrogen**
receptor antagonists)
- IT 650-51-1, Sodium trichloroacetate
RL: RCT (Reactant); RACT (Reactant or reagent)
- (ring expansion of 3-methoxy-18a-homoestra-1,3,5(10)-trien-17-
one enol silyl ether with; preparation of 17-chloro-D-homosteroids
as selective **estrogen** receptor antagonists)

L53 ANSWER 9 OF 16 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2003:298714 HCAPLUS

DOCUMENT NUMBER: 138:304438

TITLE: Preparation of 8 β -substituted
11 β -(para-substituted)aryl-estra-
2,3,5(10)-triene derivatives as contraceptives
and antiproliferatives

INVENTOR(S): Braeuer, Nico; Peters, Olaf; Hillisch,
Alexander; Hegele-hartung, Christa; Muhn,
Peter

PATENT ASSIGNEE(S): Schering AG, Germany

SOURCE: Ger. Offen., 18 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 10151114	A1	20030417	DE 2001-10151114	2001 1015
WO 2003033516	A1	20030424	WO 2002-EP11533	2002 1015

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA,
CH, CN, CO, CR, CU, CZ, DK, DM, DZ, EC, EE, ES, FI, GB,
GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP,
KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN,
MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG,
SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN,

YU, ZA, ZM, ZW
 RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
 AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ,
 DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT,
 SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML,
 MR, NE, SN, TD, TG
 US 2003171345 A1 20030911 US 2002-270077

PRIORITY APPLN. INFO.: DE 2001-10151114 A

US 2001-330728P P

2002
1015
2001
1015
2001
1029

OTHER SOURCE(S): MARPAT 138:304438
 GI

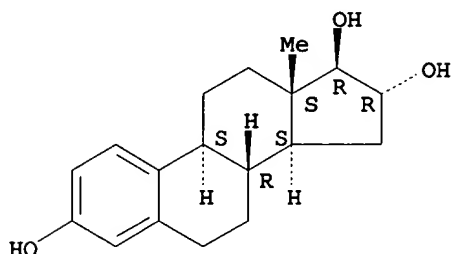
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT

AB The present invention concerns 8 β -substituted 11 β -(para-substituted)phenyl estro-1,3,5(10)-trienes, e.g., I [R2 = H, I, Br, Cl, F, OH, (un)saturated O-(C1-6-alkyl) O-(C1-6-acyl), O2CPh, OCF3, OSO2NH2, OSO2NH-alkyl, OSO2N(alkyl)2, etc.; R3 = OH, OSO2NH2, OSO2NH-alkyl, OSO2N(alkyl)2, O-aryl, O-heteroaryl, O-aralkyl, etc.; R6, R7 = H; R6' = H, OH, (un)saturated O-(C1-6-alkyl) O-(C1-6-acyl), O2CPh, OCF3, OSO2NH2, OSO2NH-alkyl, OSO2N(alkyl)2, etc.; R3 = OH, OSO2NH2, OSO2NH-alkyl, OSO2N(alkyl)2, O-aryl, O-heteroaryl, O-aralkyl, etc.; R7' = H, halogen, OH, (un)saturated O-(C1-6-alkyl) O-(C1-6-acyl), O2CPh, OCF3, OSO2NH2, OSO2NH-alkyl, OSO2N(alkyl)2, etc.; R3 = OH, OSO2NH2, OSO2NH-alkyl, OSO2N(alkyl)2, O-aryl, O-heteroaryl, O-aralkyl, etc.; R8 = straight or branched-chain, optionally partly or completely halogenated C1-5-alkyl, alkenyl, ethynyl, prop-1-ynyl; R14 = H; R14R15 = bond; R15 = H; R15R16 = bond; R15' , R16' = H, halogen, OH, (un)saturated O-(C1-6-alkyl) O-(C1-6-acyl), O2CPh, OCF3, OSO2NH2, OSO2NH-alkyl, OSO2N(alkyl)2, etc.; R3 = OH, OSO2NH2, OSO2NH-alkyl, OSO2N(alkyl)2, O-aryl, O-heteroaryl, O-aralkyl, etc.; R16 = H; R17, R17' = H, H and halogen, H and O2CPh, H and OSO2OH derivative; R17R17' = :CH-halogen, O, etc.; X = O, S, bond; Y = NH2, NH(C1-10-alkyl), N(C1-10-alkyl)2, NH(C3-7-alkyl), N(C3-7-cycloalkyl)2; Z = (CH2)n; n = 1 - 12, etc.] and their pharmaceutically acceptable salts. Thus, estratrienediol II was prepared from 3-methoxyestra-1,3,5(10)-trienone III via enol trifluoromethanesulfonylation, coupling reaction with 4-PhCH2OC6H4SnBu3, hydrogenolytic debenzoylation, etherification with N-(2-hydroxyethyl)piperidine, and acid-catalyzed hydrolysis. The new compds. are useful for the contraception with men and women, without affecting other **estrogenic**-sensitive organs like the uterus or the liver. They are suitable also for the treatment of benign or malicious proliferative illnesses of the ovary, like ovarian carcinomas and Granulosa cell tumors.

IT 50-27-1, Estriol
 RL: PAC (Pharmacological activity); THU (Therapeutic use)
 ; BIOL (Biological study); USES (Uses)
 (human **estrogen** binding ability; preparation of 8 β -substituted 11 β -(para-substituted)aryl-estra-2,3,5(10)-triene derivs. as contraceptives and antiproliferatives)
 RN 50-27-1 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16,17-triol, (16 α ,17 β)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.



IC ICM C07J001-00
ICS A61K031-565

CC 32-3 (Steroids)

Section cross-reference(s): 1, 2, 63

ST estratriene alkyl phenyl substituted prepn contraceptive antitumor
estrogen; proliferative illness treatment estratriene
alkyl phenyl substituted; ovarian carcinoma treatment estratriene
alkyl phenyl substituted; Granulosa cell tumor treatment
estratriene alkyl phenyl substituted

IT Estrogens

RL: PAC (Pharmacological activity); SPN (Synthetic preparation);
THU (Therapeutic use); BIOL (Biological study); PREP
(Preparation); USES (Uses)

(preparation of 8 β -substituted 11 β -(para-substituted)aryl-
estra-2,3,5(10)-triene derivs. as contraceptives and
antiproliferatives)

IT Estrogen receptors

RL: BSU (Biological study, unclassified); BIOL (Biological study)
(α , antagonists; preparation of 8 β -substituted
11 β -(para-substituted)aryl-estra-2,3,5(10)-triene derivs.
as contraceptives and antiproliferatives)

IT 50-27-1, Estriol 50-28-2, Estradiol, biological studies
53-16-7, Estrone, biological studies 57-91-0,
17 α -Estradiol 446-72-0, Genistein 479-13-0, Coumestrol
521-17-5, 5-Androstenediol

RL: PAC (Pharmacological activity); THU (Therapeutic use)
; BIOL (Biological study); USES (Uses)

(human estrogen binding ability; preparation of
8 β -substituted 11 β -(para-substituted)aryl-estra-
2,3,5(10)-triene derivs. as contraceptives and
antiproliferatives)

L53 ANSWER 10 OF 16 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2002:11127 HCAPLUS

DOCUMENT NUMBER: 136:64669

TITLE: Estrogenic compounds as
antiangiogenic agents

INVENTOR(S): D'Amato, Robert J.; Varma, Ravi K.; Haugwitz,
Rudiger G.; Cushman, Mark

PATENT ASSIGNEE(S): USA

SOURCE: U.S. Pat. Appl. Publ., 14 pp., Cont. of U.S.
Ser. No. 154,322, abandoned.

CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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US 2002002294

A1

20020103

US 2001-899702

2001
0705

PRIORITY APPLN. INFO.:

US 1997-59916P

P

1997
0924

US 1998-154322

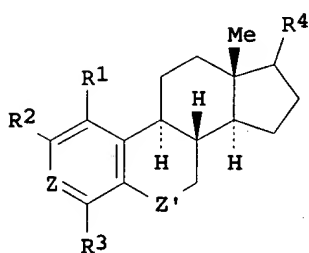
B1

1998
0916

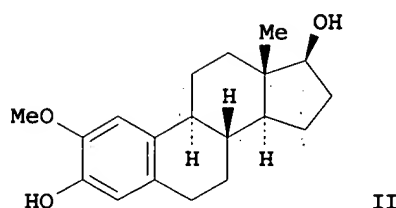
OTHER SOURCE(S):

MARPAT 136:64669

GI



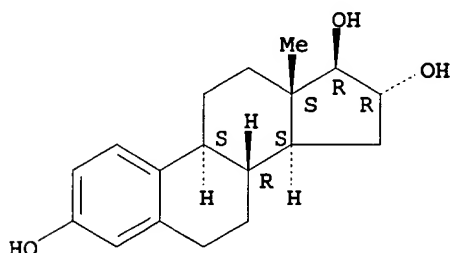
I



II

- AB 2-Methoxyestradiol derivs., such as I [R1, R3 = H, Cl, Br, I, F, CN, alkyl, OH, CH2OH, NH2, alkylamino; R2 = N3, CN, C.tplbond.CR, C=CHR, RCH=CH2, C.tplbond.CH, OR, R-R1, OR-R1 (R = alkyl, R1 = OH, NH2, Cl, Br, I, F, CF3); Z = CH, COH, CR2-OH (R2 = alkyl, aralkyl); Z' = CH2, CO, CH(OH); C=NOH, C=NOR5, CHC.tplbond.N, CHNR5R5 (R5 = H, alkyl, aralkyl)], were used for treating mammalian disease characterized by undesirable angiogenesis. Thus, 2-methoxyestradiol (II) showed inhibition of tubulin polymerization (IC50 = 3.6±0.4 μM), inhibition of colchicine binding to tubulin (1.9±0.2 μM) and antitumor activity against breast, CNS, melanoma, ovarian tumor cell assay in vitro.
- IT 50-27-1, Estriol 1236-72-2, 2-Methoxyestriol
RL: ADV (Adverse effect, including toxicity); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(estrogenic compds. as antiangiogenic agents)
- RN 50-27-1 HCAPLUS
- CN Estra-1,3,5(10)-triene-3,16,17-triol, (16α,17β)- (9CI)
(CA INDEX NAME)

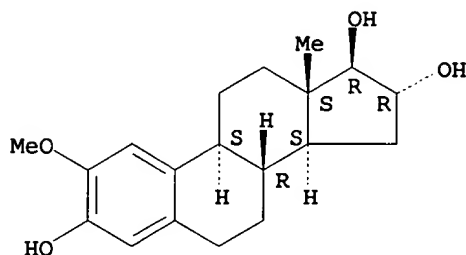
Absolute stereochemistry.



- RN 1236-72-2 HCAPLUS
- CN Estra-1,3,5(10)-triene-3,16,17-triol, 2-methoxy-,

(16 α ,17 β) - (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IC ICM C07J009-00
 ICS C07J041-00
 INCL 552009000
 CC 2-4 (Mammalian Hormones)
 Section cross-reference(s): 1, 32, 63
 ST **estrogen** antiangiogenic antitumor tubulin polymn
 inhibition; colchicine binding tubulin inhibition methoxyestradiol
 deriv
 IT Mammary gland
 (carcinoma, inhibitors; **estrogenic** compds. as
 antiangiogenic agents)
 IT Antitumor agents
 (central nervous system; **estrogenic** compds. as
 antiangiogenic agents)
 IT Nervous system
 (central, neoplasm, inhibitors; **estrogenic** compds. as
 antiangiogenic agents)
 IT Eye
 (cornea, inhibition; **estrogenic** compds. as
 antiangiogenic agents)
 IT Angiogenesis
 (**estrogenic** compds. as antiangiogenic agents)
 IT Antiestrogens
Estrogens
 RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
 (Biological study); USES (Uses)
 (**estrogenic** compds. as antiangiogenic agents)
 IT Ovary, neoplasm
 (inhibitors; **estrogenic** compds. as antiangiogenic
 agents)
 IT Antitumor agents
 (mammary gland carcinoma; **estrogenic** compds. as
 antiangiogenic agents)
 IT Antitumor agents
 (melanoma; **estrogenic** compds. as antiangiogenic
 agents)
 IT Antitumor agents
 (ovary; **estrogenic** compds. as antiangiogenic agents)
 IT Kidney, neoplasm
 (renal cell carcinoma, inhibitors; **estrogenic** compds.
 as antiangiogenic agents)
 IT Antitumor agents
 (renal cell carcinoma; **estrogenic** compds. as
 antiangiogenic agents)
 IT Structure-activity relationship
 (tubulin polymerization-inhibiting; **estrogenic** compds. as
 antiangiogenic agents)
 IT 50-27-1, Estriol 50-28-2, Estradiol, biological studies
 53-16-7, Estrone, biological studies 56-53-1, Diethylstilbestrol
 57-63-6, 17-Ethynylestradiol 64-86-8, Colchicine 362-07-2, NSC

659853 362-08-3, 2-Methoxyestrone 518-28-5, Podophyllotoxin
 1035-77-4 1236-72-2, 2-Methoxyestriol 5976-67-0,
 2-Methoxyestradiol-3-O-methyl ether 15833-07-5, 2-Bromoestradiol
 16205-32-6, 2-Fluoroestradiol 22415-44-7 26788-23-8,
 4-Methoxyestradiol 26890-04-0, 4-Methoxyestradiol-3-O-methyl
 ether 95041-90-0 117048-59-6, Combretastatin A-4
 165619-07-8, NSC 671043 165619-10-3, NSC 667049 165619-11-4,
 NSC 667047 165619-22-7, NSC 673651 165619-23-8, NSC 673652
 192062-02-5, NSC 682429 192062-12-7, NSC 679431 192062-13-8,
 NSC 681684 192062-14-9, NSC 680185 192062-15-0, NSC 681683
 192062-20-7, NSC 683125 302799-37-7, NSC 683688 383414-35-5,
 NSC 678473

RL: ADV (Adverse effect, including toxicity); PAC (Pharmacological
 activity); THU (Therapeutic use); BIOL (Biological
 study); USES (Uses)

(estrogenic compds. as antiangiogenic agents)

L53 ANSWER 11 OF 16 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2001:763027 HCAPLUS

DOCUMENT NUMBER: 135:318608

TITLE: Preparation of 8 β -hydrocarbyl-substituted
 estratrienes for use as selective
 estrogens

INVENTOR(S): Peters, Olaf; Hillisch, Alexander; Thieme,
 Ina; Elger, Walter; Hegele-Hartung, Christa;
 Kollenkirchen, Uwe; Fritzemeier,
 Karl-Heinrich; Patchev, Vladimir

PATENT ASSIGNEE(S): Schering Aktiengesellschaft, Germany

SOURCE: PCT Int. Appl., 90 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: German

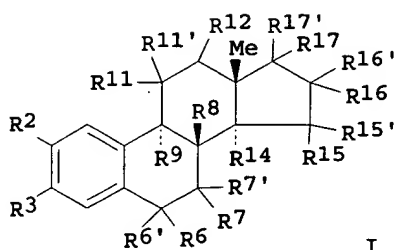
FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

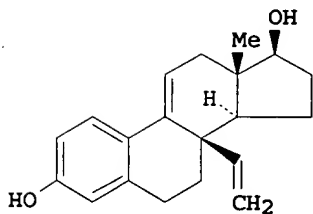
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001077139	A1	20011018	WO 2001-EP4290	2001 0412
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
DE 10019167	A1	20011018	DE 2000-10019167	2000 0412
CA 2406177	AA	20011018	CA 2001-2406177	2001 0412
EP 1272504	A1	20030108	EP 2001-931609	2001 0412
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
BR 2001009983	A	20030225	BR 2001-9983	2001 0412
JP 2003534248	T2	20031118	JP 2001-575609	

EE 200200589	A	20040415	EE 2002-589	2001 0412
ES 2245694	T3	20060116	ES 2001-1940331	2001 0412
BG 107173	A	20030530	BG 2002-107173	2001 0412
NO 2002004908	A	20021113	NO 2002-4908	2002 1008
US 2003176405	A1	20030918	US 2003-257288	2002 1011
PRIORITY APPLN. INFO.:				2003 0401
DE 2000-10019167				A 2000 0412
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WO 2001-EP4290				W 2001 0412

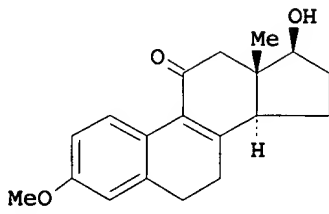
OTHER SOURCE(S): MARPAT 135:318608
GI



I



II



III

AB The invention relates to novel 8 β -substituted estratrienes I
[R2 = H, halogen, straight or branched (un)saturated C1-6-alkyl,
alkoxy, CF₃, sulfonamide; R3 = alkoxy, sulfonamide, acyloxy; R6,
R7 = H; R6R7 = bond; R6', R7' = H, halogen, alkoxy, sulfonamide;
R8 = a straight- or branched-chained, optionally partially or
completely halogenated C1-5-alkyl, alkenyl, ethynyl, prop-1-ynyl;

R9 = H, straight or branched (un)saturated C1-5-alkyl; R9R11 = bond; R11 = H; R11R12 = bond; R11' = H, halogen, a straight- or branched-chained, optionally partially or completely fluoro- or chloro-C1-4-alkyl, alkoxy, alkylthio; R12 = H; R14 = H; R14R15 = bond; R15 = H; R15R16 = bond; R15', R16' = H, halogen, alkoxy, sulfonamid; R16 = H; R17, R17' = H, H and halogen, H and OCH₂Ph, H and sulfonamide, alkyl and acyl or acyloxy, alkoxy and alkyl, alkoxy and acyloxy; R17R17' = :CH₂, :CR₂₄R₂₅; R₂₄, R₂₅ = halogen; R₂₄R₂₅ = O]. Thus, vinylestradiol II was prepared from estradiol I in 8 steps. The inventive estratrienes are used as pharmaceutically active substances that have in vitro a higher affinity to **estrogen** receptor preps. of rat prostate than to **estrogen** receptor preps. of rat uterus and which in vivo preferably have a preferential effect on bone material as compared to uterus and/or a pronounced effect with respect to the stimulation of the expression of 5HT_{2a} receptor and transporter. II showed a relative binding affinity for the **estrogen** receptor of 1 in rat uterus and of 83 in rat prostate. The invention further relates to the production of these novel compds., to their use in therapy and to the pharmaceutical forms of administration that contain said novel compds. The invention further describes the use of said compds. for treating **estrogen**-deficiency related diseases and conditions and to the use of an 8 β -substituted estratriene structural part in the overall structures of compds. that are characterized by a dissociation in favor of their **estrogen** effect on the bone as compared to the uterus.

IT 367929-22-4P 367929-25-7P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation);

THU (Therapeutic use); BIOL (Biological study); PREP

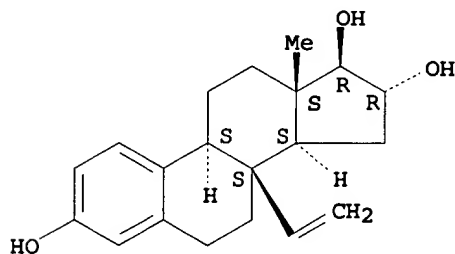
(Preparation); USES (Uses)

(preparation of 8 β -hydrocarbyl-substituted estratrienes for use as selective **estrogens**)

RN 367929-22-4 HCAPLUS

CN Estradiol-1,3,5(10)-triene-3,16,17-triol, 8-ethenyl-, (16 α ,17 β)- (9CI) (CA INDEX NAME)

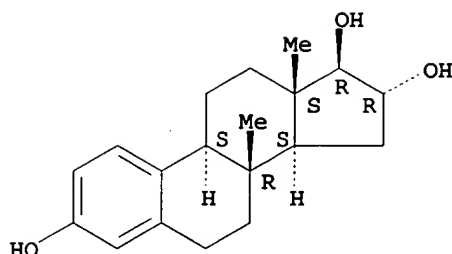
Absolute stereochemistry.



RN 367929-25-7 HCAPLUS

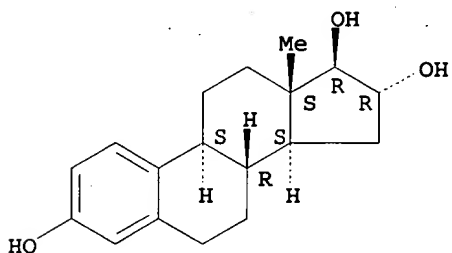
CN Estradiol-1,3,5(10)-triene-3,16,17-triol, 8-methyl-, (16 α ,17 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 50-27-1, Estriol
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use);
 BIOL (Biological study); USES (Uses)
 (preparation of 8 β -hydrocarbyl-substituted estratrienes for use as selective **estrogens**)
 RN 50-27-1 HCAPLUS
 CN Estra-1,3,5(10)-triene-3,16,17-triol, (16 α ,17 β)- (9CI)
 (CA INDEX NAME)

Absolute stereochemistry.



IC ICM C07J001-00
 ICS A61K031-565; C07J041-00; A61P005-30
 CC 32-3 (**Steroids**)
 Section cross-reference(s): 2, 63
 ST hydrocarbyl estratriene prepn **estrogen** receptor binding;
 transporter 5HT2a stimulation hydrocarbyl estratriene
 IT 5-HT receptors
 RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
 (5-HT2A, stimulation; preparation of 8 β -hydrocarbyl-substituted estratrienes for use as selective **estrogens**)
 IT **Estrogen** receptors
 RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
 (ER β ; preparation of 8 β -hydrocarbyl-substituted estratrienes for use as selective **estrogens**)
 IT Blood vessel, disease
 Heart, disease
 (circulation-related, medicaments; preparation of 8 β -hydrocarbyl-substituted estratrienes for use as selective **estrogens**)
 IT Nervous system
 (degeneration, hormone-deficiency conditioned, medicaments; preparation of 8 β -hydrocarbyl-substituted estratrienes for use as selective **estrogens**)
 IT Vagina
 (disease, atrophy, medicaments; preparation of 8 β -hydrocarbyl-substituted estratrienes for use as selective **estrogens**)
)

- IT Urogenital tract
(diseases, medicaments; preparation of 8 β -hydrocarbyl-substituted estratrienes for use as selective **estrogens**)
- IT Fertility
Sleep
(disorder, medicaments; preparation of 8 β -hydrocarbyl-substituted estratrienes for use as selective **estrogens**)
- IT Bone
Prostate gland
Uterus
(**estrogen** receptor binding in; preparation of 8 β -hydrocarbyl-substituted estratrienes for use as selective **estrogens**)
- IT Skin
(flush, hot flashes, treatment; preparation of 8 β -hydrocarbyl-substituted estratrienes for use as selective **estrogens**)
- IT Blood coagulation
(hemorrhagic diathesis, medicaments; preparation of 8 β -hydrocarbyl-substituted estratrienes for use as selective **estrogens**)
- IT Bladder
(incontinence, medicaments; preparation of 8 β -hydrocarbyl-substituted estratrienes for use as selective **estrogens**)
- IT Ovary, disease
(medicament; preparation of 8 β -hydrocarbyl-substituted estratrienes for use as selective **estrogens**)
- IT Atherosclerosis
Hyperplasia
Intestine, disease
Osteoporosis
Stomach, disease
(medicaments; preparation of 8 β -hydrocarbyl-substituted estratrienes for use as selective **estrogens**)
- IT Mental disorder
(mood-affecting, medicaments; preparation of 8 β -hydrocarbyl-substituted estratrienes for use as selective **estrogens**)
- IT Pituitary gland, anterior lobe
(neoplasm, medicaments; preparation of 8 β -hydrocarbyl-substituted estratrienes for use as selective **estrogens**)
- IT Hormone replacement therapy
(preparation of 8 β -hydrocarbyl-substituted estratrienes for use as selective **estrogens**)
- IT **Estrogens**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 8 β -hydrocarbyl-substituted estratrienes for use as selective **estrogens**)
- IT Androgens
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(replacement therapy; preparation of 8 β -hydrocarbyl-substituted estratrienes for use as selective **estrogens**)
- IT 367929-04-2P, 3-Methoxy-8 β -vinylestra-1,3,5(10)-trien-17 β -ol
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)

- (preparation of 8 β -hydrocarbyl-substituted estratrienes for use as selective **estrogens**)
- IT 26199-45-1P, 3-Methoxy-8 β -methylestra-1,3,5(10)-trien-17 β -ol 367264-86-6P 367264-89-9P 367929-00-8P, 3-Methoxy-8 β -methylestra-1,3,5(10),9(11)-tetraen-17 β -ol 367929-09-7P, 3-Methoxy-8 β -vinyl-1,3,5(10)-trien-17 α -ol 367929-14-4P, 3-Methoxy-17 α -(trifluoromethyl)-8 β -vinylestra-1,3,5(10)-trien-17 β -ol
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
- (preparation of 8 β -hydrocarbyl-substituted estratrienes for use as selective **estrogens**)
- IT 3327-97-7P, 8 β -Methylestra-1,3,5(10)-triene-3,17 β -diol 367264-78-6P 367264-79-7P 367264-81-1P 367264-83-3P 367264-85-5P 367264-87-7P 367264-90-2P 367264-92-4P 367264-95-7P 367929-01-9P, 8 β -Vinylestra-1,3,5(10),9(11)-tetraene-3,17 β -ol 367929-02-0P 367929-03-1P 367929-07-5P, 8 β -Methylestra-1,3,5(10),9(11)-tetraene-3,17 β -diol 367929-08-6P, 8 β -Ethyl-9 β -estra-1,3,5(10)-triene-3,17 β -ol 367929-10-0P, 8 β -Vinyl-1,3,5(10)-triene-3,17 α -diol 367929-11-1P, 17 α -Trifluoromethyl-8 β -vinylestra-1,3,5(10)-triene-3,17 β -diol 367929-12-2P, 8 β -Vinylestra-1,3,5(10)-triene-2,3,17 β -triol 367929-15-5P 367929-16-6P 367929-17-7P 367929-18-8P 367929-19-9P 367929-20-2P 367929-21-3P 367929-22-4P 367929-23-5P 367929-24-6P 367929-25-7P 367929-26-8P 367929-27-9P 367929-28-0P 367929-29-1P 367929-30-4P 367929-31-5P 367929-32-6P 367929-33-7P 367929-34-8P, 8 β -Vinyl-9 β -estra-1,3,5(10)-triene-3,17 β -diol
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
- (preparation of 8 β -hydrocarbyl-substituted estratrienes for use as selective **estrogens**)
- IT 50-27-1, Estriol 50-28-2, Estradiol, biological studies 53-16-7, Estrone, biological studies 57-91-0, 17 α -Estradiol 446-72-0, Genistein 479-13-0, Coumestrol 521-17-5, 5-Androstenediol
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
- (preparation of 8 β -hydrocarbyl-substituted estratrienes for use as selective **estrogens**)
- IT 1478-53-1, Diethyl (difluoromethyl)phosphonate 17401-32-0 367929-13-3, 3,17 β -Bis[(tetrahydropyran-2-yl)oxy]-8 β -vinylestra-1,3,5(10)-triene
 RL: RCT (Reactant); RACT (Reactant or reagent)
- (preparation of 8 β -hydrocarbyl-substituted estratrienes for use as selective **estrogens**)
- IT 28990-61-6P, 8 β -Formyl-3-methoxyestra-1,3,5(10),9(11)-tetraen-17 β -ol 367264-68-4P 367264-69-5P 367264-70-8P 367264-71-9P 367264-72-0P 367264-73-1P 367264-74-2P 367264-75-3P 367264-76-4P 367264-77-5P 367264-80-0P 367264-82-2P 367264-84-4P 367264-88-8P 367264-91-3P 367264-93-5P 367264-94-6P 367264-96-8P 367279-41-2P 367929-05-3P, 3-Methoxy-8 β -vinylestra-1,3,5(10)-trien-17-one 367929-06-4P, 3-Hydroxy-8 β -vinylestra-1,3,5(10)-trien-17-one
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
- (preparation of 8 β -hydrocarbyl-substituted estratrienes for use as selective **estrogens**)

REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE

FOR THIS RECORD. ALL CITATIONS AVAILABLE
IN THE RE FORMAT

L53 ANSWER 12 OF 16 HCAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 2001:763026 HCAPLUS
 DOCUMENT NUMBER: 135:318607
 TITLE: Preparation of 8 β -substituted-11 β -
 pentyl- and 11 β -hexyl-estra-1,3,5(10)-
 triene derivatives which have an affinity for
 the **estrogen** receptor
 INVENTOR(S): Peters, Olaf; Braeuer, Nico; Hillisch,
 Alexander; Hegele-Hartung, Christa;
 Fritzemeier, Karl-Heinrich
 PATENT ASSIGNEE(S): Schering Aktiengesellschaft, Germany
 SOURCE: PCT Int. Appl., 53 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 2
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001077138	A1	20011018	WO 2001-EP4289	2001 0412
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CO, CR, CU, CZ, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
DE 10019167	A1	20011018	DE 2000-10019167	2000 0412
EP 1272505	A1	20030108	EP 2001-940331	2001 0412
EP 1272505	B1	20050824		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2003530403	T2	20031014	JP 2001-575608	2001 0412
AT 302790	E	20050915	AT 2001-940331	2001 0412
ES 2245694	T3	20060116	ES 2001-1940331	2001 0412
NO 2002004907	A	20021205	NO 2002-4907	2002 1011
US 2004029847	A1	20040212	US 2003-257287	2003 0708
PRIORITY APPLN. INFO.:				A
DE 2000-10019167				2000 0412
US 2000-207370P				P

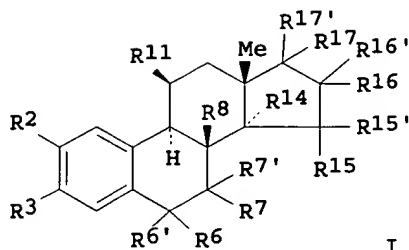
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WO 2001-EP4289

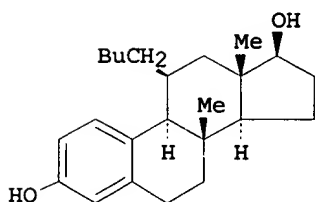
W

2001
0412OTHER SOURCE(S):
GI

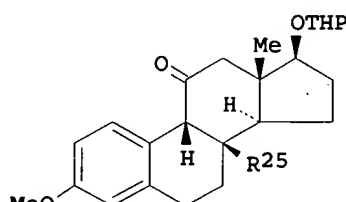
MARPAT 135:318607



I



II



III

AB The present invention relates to the novel 8β -substituted estradienes I [R2 = H, F, Cl, Br, I, straight or branched (un)saturated C1-6-alkyl, OH, alkoxy, acyloxy, CF3, sulfamoyloxy; R3 = alkoxy, sulfamoyloxy, acyloxy; R6, R6' = H; R6R7 = bond; R7, R7' = H; R8 means a straight-chain or branched-chain, optionally partially or entirely halogenated alkyl or alkenyl radical having up to 5 carbon atoms, an ethynyl or prop-1-ynyl radical; R11 = pentyl, hexyl; R14 = H; R14R15 = bond; R15 = H; R15', R16' = H, F, Cl, Br, I, alkoxy, sulfamoyloxy, acyloxy; R15R16 = bond; R16 = H; R17, R17' = H, H and halogen, H and OCH2Ph, H and sulfamoyloxy; alkyl and acyl or acyloxy; alkoxy and alkyl, alkoxy and acyloxy; R17R17' = CH2 CR23R24; R23, R24 = H, halogen; R23R24 = O]. Thus, 8β -methyl- 11β -pentyl-1,3,5(10)-triene-3,17 β -diol (II) was prepared from 8β -cyanosteroid III (R25 = CN) via condensation of 11-ketosteroid III (R25 = Me) with BuCH2Li. Estradienes I are used as pharmaceutical active agents which, in vitro, are provided with a higher affinity of **estrogen** receptor preps. of rat prostate than of **estrogen** receptor preps. of rat uterus and, in vivo, preferably act in a preferential contraceptive manner on the ovary without stimulating the uterus. The invention also relates to the production thereof, the therapeutic use thereof and pharmaceutical administration forms which contain the novel compds. I. The invention further relates to the use of compds. I for male contraception and to the use of non-malignant or malignant proliferate diseases of the ovary, such as ovarian carcinoma or granulosa cell tumors for instance.

IT 50-27-1, Estriol

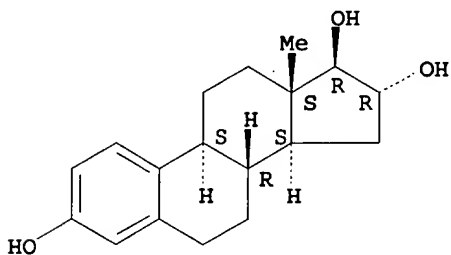
RL: BAC (Biological activity or effector, except adverse); BSU

(Biological study, unclassified); THU (Therapeutic use);
 BIOL (Biological study); USES (Uses)
 (preparation of 8 β -substituted-11 β -pentyl- and
 -11 β -hexyl-estra-1,3,5(10)-triene derivs. which have an
 affinity for the **estrogen** receptor)

RN 50-27-1 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16,17-triol, (16 α ,17 β)- (9CI)
 (CA INDEX NAME)

Absolute stereochemistry.



IC ICM C07J001-00

ICS A61K031-565; C07J041-00; A61P005-30

CC 32-3 (Steroids)

Section cross-reference(s): 1, 2, 63

ST estratriene pentyl hexyl deriv prepn **estrogen** receptor
 binding affinity; contraceptive estratriene pentyl hexyl deriv
 prepn; ovarian proliferate disease inhibitor estratriene pentyl
 hexyl deriv prepn; granulosa cell tumor inhibitor estratriene
 pentyl hexyl deriv prepn

IT Hormone replacement therapy

(GnHR antagonists; preparation of 8 β -substituted-11 β -
 pentyl- and -11 β -hexyl-estra-1,3,5(10)-triene derivs.
 which have an affinity for the **estrogen** receptor)

IT Progesterone receptors

RL: BPR (Biological process); BSU (Biological study,
 unclassified); BIOL (Biological study); PROC (Process)
 (antagonists; preparation of 8 β -substituted-11 β -pentyl-
 and -11 β -hexyl-estra-1,3,5(10)-triene derivs. which have
 an affinity for the **estrogen** receptor)

IT Ovary, neoplasm

(carcinoma, inhibitors; preparation of 8 β -substituted-11 β -
 pentyl- and -11 β -hexyl-estra-1,3,5(10)-triene derivs.
 which have an affinity for the **estrogen** receptor)

IT Ovary

(contraceptives affecting; preparation of 8 β -substituted-
 11 β -pentyl- and -11 β -hexyl-estra-1,3,5(10)-triene
 derivs. which have an affinity for the **estrogen**
 receptor)

IT Prostate gland

Uterus

(**estrogen** receptor affinity; preparation of
 8 β -substituted-11 β -pentyl- and -11 β -hexyl-estra-
 1,3,5(10)-triene derivs. which have an affinity for the
estrogen receptor)

IT Contraceptives

(female; preparation of 8 β -substituted-11 β -pentyl- and
 -11 β -hexyl-estra-1,3,5(10)-triene derivs. which have an
 affinity for the **estrogen** receptor)

IT Progestogens

RL: BAC (Biological activity or effector, except adverse); BSU
 (Biological study, unclassified); RCT (Reactant); SPN (Synthetic
 preparation); THU (Therapeutic use); BIOL (Biological study); PREP
 (Preparation); RACT (Reactant or reagent); USES (Uses)

- (gestagens and mesoproggestins; preparation of 8 β -substituted-11 β -pentyl- and -11 β -hexyl-estra-1,3,5(10)-triene derivs. which have an affinity for the **estrogen** receptor)
- IT Ovary, neoplasm
(granulosa cell tumor, inhibitors; preparation of 8 β -substituted-11 β -pentyl- and -11 β -hexyl-estra-1,3,5(10)-triene derivs. which have an affinity for the **estrogen** receptor)
- IT Antitumor agents
(granulosa cell tumor; preparation of 8 β -substituted-11 β -pentyl- and -11 β -hexyl-estra-1,3,5(10)-triene derivs. which have an affinity for the **estrogen** receptor)
- IT Contraceptives
(male; preparation of 8 β -substituted-11 β -pentyl- and -11 β -hexyl-estra-1,3,5(10)-triene derivs. which have an affinity for the **estrogen** receptor)
- IT Antitumor agents
(ovary carcinoma; preparation of 8 β -substituted-11 β -pentyl- and -11 β -hexyl-estra-1,3,5(10)-triene derivs. which have an affinity for the **estrogen** receptor)
- IT **Estrogens**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of 8 β -substituted-11 β -pentyl- and -11 β -hexyl-estra-1,3,5(10)-triene derivs. which have an affinity for the **estrogen** receptor)
- IT **Estrogen receptors**
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(preparation of 8 β -substituted-11 β -pentyl- and -11 β -hexyl-estra-1,3,5(10)-triene derivs. which have an affinity for the **estrogen** receptor)
- IT Disease, animal
(proliferative, ovarian, inhibitors; preparation of 8 β -substituted-11 β -pentyl- and -11 β -hexyl-estra-1,3,5(10)-triene derivs. which have an affinity for the **estrogen** receptor)
- IT 367269-62-3P, 3-Methoxy-8 β -methyl-11-pentylestra-1,3,5(10),9(11)-tetraen-17 β -ol 367269-63-4P, 11-Hexyl-3-methoxy-8 β -methylestra-1,3,5(10),9(11)-tetraen-17 β -ol 367269-64-5P, 3-Methoxy-8 β -methyl-11 β -pentylestra-1,3,5(10)-trien-17 β -ol 367269-65-6P, 11 β -Hexyl-3-methoxy-8 β -methylestra-1,3,5(10)-trien-17 β -ol 367269-77-0P, 3-Methoxy-11 β -pentyl-8 β -vinylestra-1,3,5(10)-trien-17 β -ol 367269-78-1P, 11 β -Hexyl-3-methoxy-8 β -vinylestra-1,3,5(10)-trien-17 β -ol
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of 8 β -substituted-11 β -pentyl- and -11 β -hexyl-estra-1,3,5(10)-triene derivs. which have an affinity for the **estrogen** receptor)
- IT 367269-66-7P, 8 β -Methyl-11 β -pentylestra-1,3,5(10)-triene-3,17 β -diol 367269-67-8P, 11 β -Hexyl-8 β -methylestra-1,3,5(10)-triene-3,17 β -diol 367269-79-2P, 11 β -Pentyl-8 β -vinylestra-1,3,5(10)-triene-3,17 β -diol 367269-80-5P, 11 β -Hexyl-8 β -vinylestra-1,3,5(10)-triene-3,17 β -diol 367269-81-6P, 8 β -Ethyl-11 β -pentyl-1,3,5(10)-triene-3,17 β -diol 367269-82-7P, 8 β -Ethyl-11 β -hexyl-1,3,5(10)-triene-3,17 β -diol 367269-83-8P, 8 β -Methyl-11 β -pentyl-1,3,5(10)-triene-

3,17 β -diol 3-sulfamate 367269-84-9P, 8 β -Ethyl-11 β -
 pentyl-1,3,5(10)-triene-3,17 β -diol 3-sulfamate
 367269-85-0P, 11 β -Pentyl-8 β -vinyl-1,3,5(10)-triene-
 3,17 β -diol 3-sulfamate 367269-86-1P, 11 β -Hexyl-8 β -
 methyl-1,3,5(10)-triene-3,17 β -diol 3-sulfamate
 367269-87-2P, 8 β -Ethyl-11 β -hexyl-1,3,5(10)-triene-
 3,17 β -diol 3-sulfamate 367269-88-3P, 11 β -Hexyl-8 β -
 vinyl-1,3,5(10)-triene-3,17 β -diol 3-sulfamate 367269-89-4P,
 8 β -Methyl-11 β -pentyl-1,3,5(10)-triene-3,17 β -diol
 3-acetate 367269-90-7P, 8 β -Ethyl-11 β -pentyl-1,3,5(10)-
 triene-3,17 β -diol 3-acetate 367269-91-8P,
 11 β -Pentyl-8 β -vinyl-1,3,5(10)-triene-3,17 β -diol
 3-acetate 367269-92-9P, 11 β -Hexyl-8 β -methyl-1,3,5(10)-
 triene-3,17 β -diol 3-acetate 367269-93-0P,
 8 β -Ethyl-11 β -hexyl-1,3,5(10)-triene-3,17 β -diol
 3-acetate 367269-94-1P, 11 β -Hexyl-8 β -vinyl-1,3,5(10)-
 triene-3,17 β -diol 3-acetate

RL: BAC (Biological activity or effector, except adverse); BSU
 (Biological study, unclassified); SPN (Synthetic preparation); THU
 (Therapeutic use); BIOL (Biological study); PREP (Preparation);
 USES (Uses)

(preparation of 8 β -substituted-11 β -pentyl- and
 -11 β -hexyl-estra-1,3,5(10)-triene derivs. which have an
 affinity for the **estrogen** receptor)

IT 50-27-1, Estriol 50-28-2; Estradiol, biological studies
 53-16-7, Estrone, biological studies 57-91-0,
 17 α -Estradiol 446-72-0, Genistein 479-13-0, Coumestrol
 521-17-5, 5-Androstenediol

RL: BAC (Biological activity or effector, except adverse); BSU
 (Biological study, unclassified); THU (Therapeutic use);
 BIOL (Biological study); USES (Uses)

(preparation of 8 β -substituted-11 β -pentyl- and
 -11 β -hexyl-estra-1,3,5(10)-triene derivs. which have an
 affinity for the **estrogen** receptor)

IT 3525-31-3, Pentyllithium 21369-64-2, Hexyllithium 367269-56-5
 367269-68-9

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of 8 β -substituted-11 β -pentyl- and
 -11 β -hexyl-estra-1,3,5(10)-triene derivs. which have an
 affinity for the **estrogen** receptor)

IT 367269-57-6P 367269-58-7P 367269-59-8P 367269-60-1P
 367269-61-2P 367269-69-0P 367269-70-3P 367269-71-4P,
 8 β -Cyano-3-methoxy-11 β -pentylestra-1,3,5(10,9(11))-
 tetraen-17 β -ol 367269-72-5P, 8 β -Cyano-11 β -hexyl-3-
 methoxyestra-1,3,5(10,9(11))-tetraen-17 β -ol 367269-73-6P,
 8 β -Formyl-3-methoxy-11 β -pentylestra-1,3,5(10,9(11))-
 tetraen-17 β -ol 367269-74-7P, 8 β -Formyl-11 β -hexyl-
 3-methoxyestra-1,3,5(10,9(11))-tetraen-17 β -ol 367269-75-8P,
 8 β -Formyl-3-methoxy-11 β -pentylestra-1,3,5(10)-trien-
 17 β -ol 367269-76-9P, 8 β -Formyl-11 β -hexyl-3-
 methoxyestra-1,3,5(10)-trien-17 β -ol

RL: RCT (Reactant); SPN (Synthetic preparation); PREP
 (Preparation); RACT (Reactant or reagent)

(preparation of 8 β -substituted-11 β -pentyl- and
 -11 β -hexyl-estra-1,3,5(10)-triene derivs. which have an
 affinity for the **estrogen** receptor)

REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE
 FOR THIS RECORD. ALL CITATIONS AVAILABLE
 IN THE RE FORMAT

L53 ANSWER 13 OF 16 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1997:192107 HCAPLUS

DOCUMENT NUMBER: 126:190942

TITLE: Transdermal administration of esters of
 13-ethyl-17 β -hydroxy-11-methylene-18,19-
 dinor-17- α -pregn-4-en-20-yn-3-one

INVENTOR(S): Lipp, Ralph; Ewers, Christian L. J.; Guenther, Clemens; Riedl, Jutta; Taeuber, Ulrich
 PATENT ASSIGNEE(S): Schering A.-G., Germany
 SOURCE: Ger. Offen., 11 pp.
 CODEN: GWXXBX
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 19613698	A1	19970123	DE 1996-19613698	1996 0401
WO 9703709	A1	19970206	WO 1996-EP3033	1996 0706
W: AU, BR, CA, CN, CZ, FI, HU, IL, JP, KR, MX, NO, NZ, PL, RU, SK, UA, US, VN				
RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
AU 9666140	A1	19970218	AU 1996-66140	1996 0706
EP 848620	A1	19980624	EP 1996-925717	1996 0706
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
JP 11509222	T2	19990817	JP 1996-506250	1996 0706
ZA 9606083	A	19980619	ZA 1996-6083	1996 0717
PRIORITY APPLN. INFO.:			DE 1995-19526789	A1 1995 0717
			DE 1996-19613698	A 1996 0401
			WO 1996-EP3033	W 1996 0706

AB The title compds. in combination with 1 or more **estrogens** are suitable for the transdermal administration and therapy of diseases such as osteoporosis. Thus, 0.8 g 13-ethyl-17 β -hexanoyloxy-11-methylene-18,19-dinor-17- α -pregn-4-en-20-yn-3-one (preparation method given) and 8.0 g dimethylisosorbide were mixed in 62.4 g 50% solution of silicone rubber in petrol. This mixture was coated on a polyester film and the laminate could be used for transdermal hormone delivery.

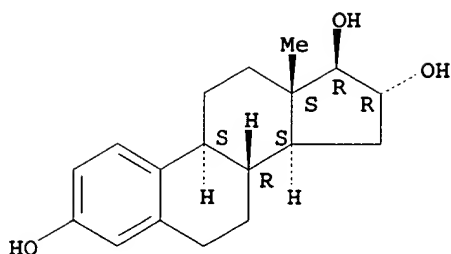
IT 50-27-1, Estriol 187538-69-8
 RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(transdermal administration of dinorpregnynone esters)

RN 50-27-1 HCAPLUS

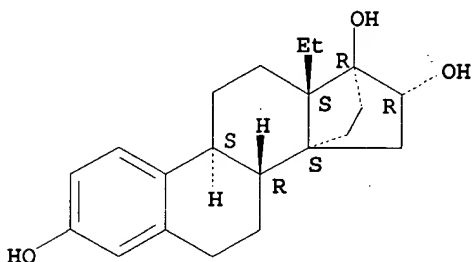
CN Estra-1,3,5(10)-triene-3,16,17-triol, (16 α ,17 β)- (9CI)
 (CA INDEX NAME)

Absolute stereochemistry.



RN 187538-69-8 HCAPLUS
 CN 14,21-Cyclo-18,19-dinorpregna-1,3,5(10)-triene-3,16,17-triol,
 13-ethyl-, (16 α ,17 α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IC ICM C07J001-00
 ICS A61K031-565; A61L015-44
 CC 63-6 (Pharmaceuticals)
 Section cross-reference(s): 2, 32
 ST dinorpregnynone ester **estrogen** transdermal prepn
 IT **Estrogens**
 Osteoporosis
 Ovarian cycle
 RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
 (transdermal administration of dinorpregnynone esters)
 IT 50-27-1, Estriol 50-28-2, Estradiol, biological studies
 57-63-6, 17 α -EthinylEstradiol 72-33-3, Mestranol
 54048-10-1 54048-10-1D, esters 187538-68-7 187538-69-8
 RL: THU (Therapeutic use); BIOL (Biological study); USES
 (Uses)
 (transdermal administration of dinorpregnynone esters)

L53 ANSWER 14 OF 16 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1992:612787 HCAPLUS

DOCUMENT NUMBER: 117:212787

TITLE: Preparation and formulation of
 [bis(phosphono)butylaminocarbonyloxylestratrie
 ne and analogs for treatment of bone disease
 INVENTOR(S): Saari, Walfred S.; Rodan, Gideon A.; Fisher,
 Thorsten E.; Anderson, Paul S.

PATENT ASSIGNEE(S): Merck and Co., Inc., USA

SOURCE: Eur. Pat. Appl., 21 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

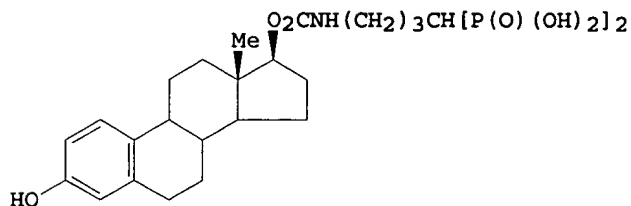
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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OTHER SOURCE(S) : MARPAT 117:212787
GI



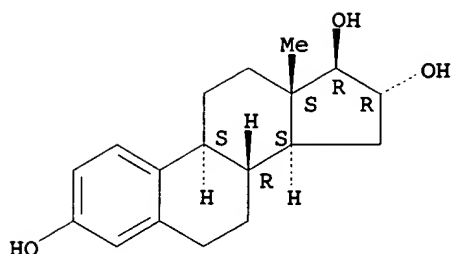
AB Comps. ABC [A = residue of a hydroxy-containing steroidal hormone having human bone resorption-antagonist activity or bone formation-stimulatory activity; C = residue of an amino- or hydroxyalkyl-1,1-bis(phosphonate) having human bone affinity; B = covalent linkage connecting A through the hydroxyl moiety and C through the amino or hydroxyl moiety, which linkage can hydrolyze in the human body in the vicinity of bone to release steroidal hormone A] were prepared for treatment of bone disorders (no data). Thus, [(Me2CHO)2P(O)]2CHR (I; R = H), was condensed with CH2:CHCN and the product hydrogenated to give I [R = (CH2)3NH2], which was condensed with 3-benzyloxy-17 β -chlorocarbonyloxyestra-1,3,5(10)-triene (preparation given) to give, after deprotection, title compound II.

IT 50-27-1DP, derivs. linked to bisphosphonate moieties
RL: THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, for treatment of bone disease)

RN 50-27-1 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16,17-triol, (16 α ,17 β)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.



IC ICM C07J051-00

ICS A61K031-565; C07F009-40

CC 32-3 (Steroids)

Section cross-reference(s): 1, 29, 63

IT 50-02-2DP, derivs. linked to bisphosphonate moieties 50-03-3DP, derivs. linked to bisphosphonate moieties 50-22-6DP, derivs. linked to bisphosphonate moieties 50-23-7DP, derivs. linked to bisphosphonate moieties 50-24-8DP, derivs. linked to bisphosphonate moieties 50-27-1DP, derivs. linked to bisphosphonate moieties 50-28-2DP, Estra-1,3,5(10)-triene-3,17-diol (17 β)-, derivs. linked to bisphosphonate moieties 50-50-0DP, derivs. linked to bisphosphonate moieties 52-76-6DP, derivs. linked to bisphosphonate moieties 52-78-8DP, derivs. linked to bisphosphonate moieties 53-03-2DP, derivs. linked to bisphosphonate moieties 53-06-5DP, derivs. linked to bisphosphonate moieties 53-33-8DP, derivs. linked to bisphosphonate moieties 53-34-9DP, derivs. linked to bisphosphonate moieties 53-39-4DP, derivs. linked to bisphosphonate moieties 53-41-8DP, derivs. linked to bisphosphonate moieties 53-43-0DP, derivs. linked to bisphosphonate moieties 57-63-6DP, derivs. linked to bisphosphonate moieties 58-18-4DP, derivs. linked to bisphosphonate moieties 58-22-0DP, derivs. linked to bisphosphonate moieties 67-73-2DP, derivs. linked to bisphosphonate moieties 67-81-2DP, derivs. linked to bisphosphonate moieties 68-22-4DP, derivs. linked to bisphosphonate moieties 68-23-5DP, derivs. linked to bisphosphonate moieties 68-96-2DP, derivs. linked to bisphosphonate moieties 72-33-3DP, derivs. linked to bisphosphonate moieties 72-63-9DP, derivs. linked to bisphosphonate moieties 76-25-5DP, derivs. linked to bisphosphonate moieties 76-43-7DP, derivs. linked to bisphosphonate moieties 76-47-1DP, derivs. linked to bisphosphonate moieties 79-64-1DP, derivs. linked to bisphosphonate moieties 83-43-2DP, derivs. linked to bisphosphonate moieties 124-94-7DP, derivs. linked to bisphosphonate moieties 125-02-0DP, derivs. linked to bisphosphonate moieties 125-04-2DP, derivs. linked to bisphosphonate moieties 145-12-0DP, derivs. linked to bisphosphonate moieties 152-43-2DP, derivs. linked to bisphosphonate moieties 152-97-6DP, derivs. linked to bisphosphonate moieties 153-00-4DP, derivs. linked to bisphosphonate moieties 356-12-7DP, derivs. linked to bisphosphonate moieties 360-66-7DP, derivs. linked to bisphosphonate moieties 378-44-9DP, derivs. linked to bisphosphonate moieties 382-67-2DP, derivs. linked to bisphosphonate moieties 426-13-1DP, derivs. linked to bisphosphonate moieties 432-60-0DP, derivs. linked to bisphosphonate moieties 434-03-7DP, derivs. linked to bisphosphonate moieties 434-07-1DP, derivs. linked to bisphosphonate moieties 434-22-0DP, derivs. linked to bisphosphonate moieties 471-53-4DP, derivs. linked to bisphosphonate moieties 474-86-2DP, derivs. linked to

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 bisphosphonate moieties

RL: THU (Therapeutic use); BIOL (Biological study); PREP
 (Preparation); USES (Uses)
 (preparation of, for treatment of bone disease)

L53 ANSWER 15 OF 16 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1987:5325 HCAPLUS
 DOCUMENT NUMBER: 106:5325
 TITLE: Estradiol and estriol glycolates
 INVENTOR(S): Duesterberg, Bernd; Acksteiner, Bernard;
 Schulze, Paul Eberhard
 PATENT ASSIGNEE(S): Schering A.-G., Fed. Rep. Ger.
 SOURCE: Ger. Offen., 12 pp.
 CODEN: GWXXBX
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3511587	A1	19861002	DE 1985-3511587	1985 0327
EP 196271	A2	19861001	EP 1986-730052	1986 0320
EP 196271	A3	19870204		
EP 196271	B1	19890208		
R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE				
AT 40695	E	19890215	AT 1986-730052	1986 0320
JP 61221198	A2	19861001	JP 1986-67418	1986 0327
US 4780460	A	19881025	US 1986-845102	1986 0327
PRIORITY APPLN. INFO.:			DE 1985-3511587	A 1985 0327
			EP 1986-730052	A 1986 0320

OTHER SOURCE(S): CASREACT 106:5325; MARPAT 106:5325

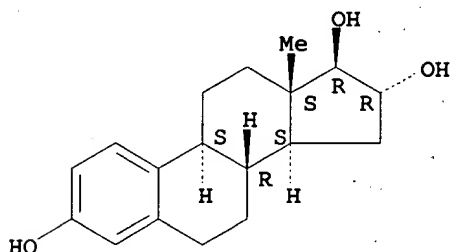
AB Title esters RO₂CCH₂Z (R = residue of estradiol or estriol; Z = OH, O₂CR₁; R₁ = Me, Ph) are prepared as **estrogens** (no data), usable as aqueous crystalline suspensions in long-acting injectable contraceptives. Thus, esterification of estradiol with PhCO₂CH₂COCl in C₂Cl₄ in the presence of collidine gave estradiol 3,17 β -bis(benzoyloxyacetate), which was saponified to give estradiol 17 β -benzoyloxyacetate (I). An injectable 1-mL saline suspension containing microcryst. I and norethisterone 17 β -benzoyloxyacetate was prepared as a 1-mo contraceptive.

IT 50-27-1, Estriol
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (esterification of, with acetoxyacetyl and benzoyloxyacetyl chlorides)

RN 50-27-1 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16,17-triol, (16 α ,17 β)- (9CI)
 (CA INDEX NAME)

Absolute stereochemistry.



IC ICM C07J001-00
 ICS A61K031-565

CC 32-3 (**Steroids**)
 Section cross-reference(s): 2, 63

ST glycolate estradiol estriol prepn **estrogen**;
 contraceptive estradiol estriol glycolate prepn; injection
 contraceptive estradiol estriol glycolate

IT **Estrogens**
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (estradiol and estriol glycolates)

IT 50-27-1, Estriol 50-28-2, Estradiol, reactions
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (esterification of, with acetoxyacetyl and benzoyloxyacetyl chlorides)

IT 105426-11-7P, Estradiol 17 β -benzoyloxyacetate 105579-76-8P,
 Estradiol 3,17 β -bis(acetoxyacetate) 105579-77-9P, Estradiol
 17 β -acetoxyacetate 105579-78-0P, Estradiol
 17 β -glycolate 105579-79-1P 105579-80-4P, Estriol
 3,16 α ,17 β -tris(acetoxyacetate) 105579-81-5P, Estriol
 16 α ,17 β -bis(acetoxyacetate) 105579-82-6P
 105579-83-7P, Estriol 16 α ,17 β -bis(benzoyloxyacetate)
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of, as **estrogen**)

L53 ANSWER 16 OF 16 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1975:175239 HCAPLUS

DOCUMENT NUMBER: 82:175239

TITLE: 17 α -Ethinylestriol-3-cyclopentyl ether

INVENTOR(S): Kraay, Russell J.; Farkas, Eugene

PATENT ASSIGNEE(S): Eli Lilly and Co., USA

SOURCE: U.S., 7 pp. Division of U.S. 3,790,605 (CA 80;121211e).
 CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 5
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3868452	A	19750225	US 1973-411988	1973 1101
US 3790605	A	19740205	US 1971-136671	1971 0423
PRIORITY APPLN. INFO.:			US 1971-127690	A2 1971 0324
			US 1971-136671	A3 1971 0423

GI For diagram(s), see printed CA Issue.

AB 17 α -Ethinylestriol 3-cyclopentyl ether (I) [39791-20-3], a potent **estrogen** was useful in doses of 5-500 μ g/day in treatment of menopausal syndrome and other conditions of **estrogen** deficiency or in which **estrogens** may be used therapeutically. 16 α -Hydroxyestrone diacetate [1247-71-8] treated with ethynylmagnesium bromide gave 17 α -ethinylestriol [4717-40-2] and the 17 β -isomer [10098-79-0]. Elution with MeOH, washing with CHCl₃ and recrystn. from EtOAc-hexane mixture gave pure α -isomer, which was converted to Na salt [53154-93-1]. Treatment with cyclopentyl bromide [137-43-9] in formamide solution gave I, recrystd. from ether-hexane mixture, m. about 162-5°. Pharmacol. tests and pharmaceutical formulations were given.

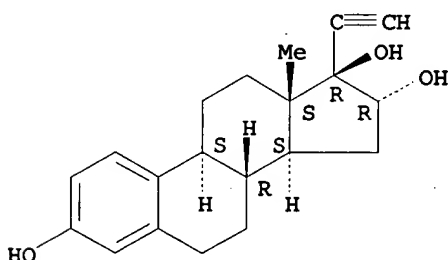
IT 53154-93-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and reaction with cyclopentyl bromide)

RN 53154-93-1 HCAPLUS

CN 19-Norpregna-1,3,5(10)-trien-20-yne-3,16,17-triol, monosodium salt, (16 α ,17 α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



● Na

IT 4717-40-2P

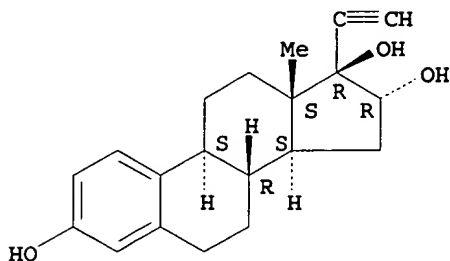
RL: PREP (Preparation) (preparation and sodium salt formation of)

RN 4717-40-2 HCAPLUS

CN 19-Norpregna-1,3,5(10)-trien-20-yne-3,16,17-triol,

(16 α ,17 α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



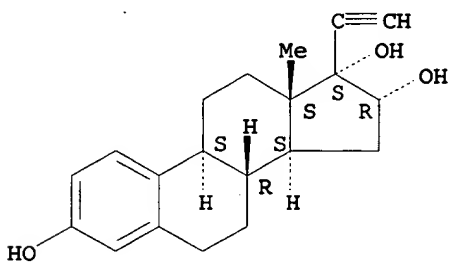
IT 10098-79-0P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 10098-79-0 HCAPLUS

CN 19-Norpregna-1,3,5(10)-trien-20-yne-3,16,17-triol, (16 α)-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.



IC A61K

INCL 424238000

CC 63-6 (Pharmaceuticals)

Section cross-reference(s): 2, 32

IT 53154-93-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP
(Preparation); RACT (Reactant or reagent)
(preparation and reaction with cyclopentyl bromide)

IT 4717-40-2P

RL: PREP (Preparation)
(preparation and sodium salt formation of)

IT 10098-79-0P 39791-18-9P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

=> => d que stat 156

L12 289 SEA FILE=REGISTRY ABB=ON PLU=ON (10449-00-0/BI OR
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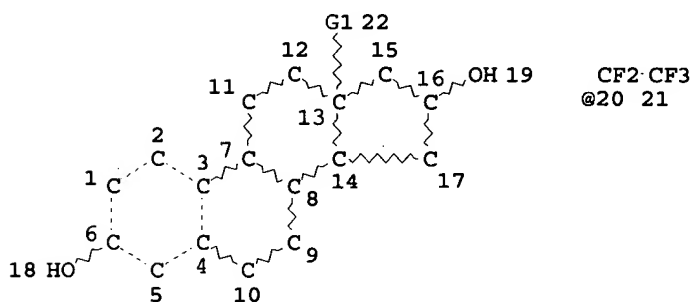
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 287722-46-7/BI OR 287722-47-8/BI OR 287722-4

L13

L14

SCR 1844

STR



VAR G1=ME/ET/CF3/20

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 22

STEREO ATTRIBUTES: NONE

L15 899 SEA FILE=REGISTRY SSS FUL L14 NOT L13

L16 266 SEA FILE=REGISTRY ABB=ON PLU=ON L12 AND L15

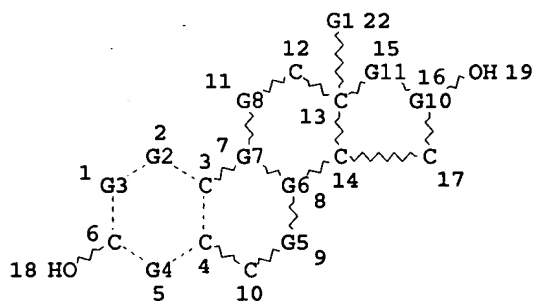
L25 STR

CF2·CF3 C~X C~CF3 C~OH C~Me C~OMe
 @20 21 @23 24 @25 26 @27 28 @29 30 @31 32

C~OEt C~Ak C~O~Ak C~CF2·CF3 C~Ak~F
 @33 34 @35 36 @37 38 39 @42 41 40 @43 44 45

C~Cy C~CN C~Et C~O~NO2 C~CH2Cl
 @46 47 @48 49 @50 51 @52 53 54 @55 56 57

C~G9 C~S~Ak S @62
 @58 59 @60 61 63



C~CH2·CN C~F
 @64 65 66 @67 68

VAR G1=ME/ET/CF3/20
 VAR G2=CH/23/27/25/29/31/33
 VAR G3=CH/23/27/35/37
 VAR G4=CH/23/35/25/42/37
 VAR G5=CH/23/35/43/37/46
 VAR G6=CH/35/43/48
 VAR G7=CH/29/50/25/42
 VAR G8=CH2/CH/52/27/58/23/55/35/43/37/46
 VAR G9=62/60
 VAR G10=CH/35/43/25/42/64
 VAR G11=CH2/CH/67/35/43

NODE ATTRIBUTES:

CONNECT IS E2 RC AT 61
 CONNECT IS E1 RC AT 62
 DEFAULT MLEVEL IS ATOM
 GGCAT IS UNS AT 47
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 68

STEREO ATTRIBUTES: NONE

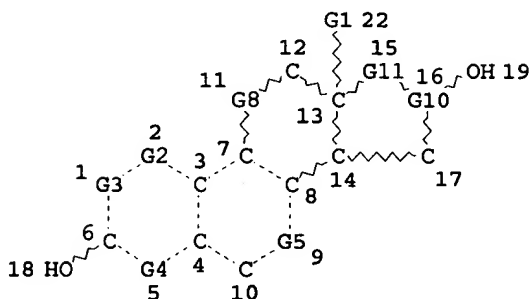
L26 STR

CF2 CF3 C~X C~CF3 C~OH C~Me C~OMe
 @20 21 @23 24 @25 26 @27 28 @29 30 @31 32

C~OEt C~Ak C~O~Ak C~CF2 CF3 C~Ak~F
 @33 34 @35 36 @37 38 39 @42 41 40 @43 44 45

C~Cy C~CN C~Et C~O~NO2 C~CH2Cl
 @46 47 48 49 50 51 @52 53 54 @55 56 57

C~G9 C~S~Ak S @62
 @58 59 @60 61 63



C~CH2-CN C~F
 @64 65 66 @67 68

VAR G1=ME/ET/CF3/20
 VAR G2=CH/23/27/25/29/31/33
 VAR G3=CH/23/27/35/37
 VAR G4=CH/23/35/25/42/37
 VAR G5=CH/23/35/43/37/46
 VAR G8=CH2/CH/52/27/58/23/55/35/43/37/46
 VAR G9=62/60
 VAR G10=CH/35/43/25/42/64
 VAR G11=CH2/CH/67/35/43

NODE ATTRIBUTES:

CONNECT IS E2 RC AT 61
 CONNECT IS E1 RC AT 62
 DEFAULT MLEVEL IS ATOM
 GGCAT IS UNS AT 47
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 68

STEREO ATTRIBUTES: NONE

L28 631 SEA FILE=REGISTRY SUB=L15 SSS FUL (L25 OR L26)
 L31 6412 SEA FILE=HCAPLUS ABB=ON PLU=ON L15
 L32 6195 SEA FILE=HCAPLUS ABB=ON PLU=ON L28
 L33 24 SEA FILE=HCAPLUS ABB=ON PLU=ON L16
 L34 46181 SEA FILE=HCAPLUS ABB=ON PLU=ON STEROID?/SC,SX
 L35 362 SEA FILE=HCAPLUS ABB=ON PLU=ON L31 AND L34
 L36 316 SEA FILE=HCAPLUS ABB=ON PLU=ON L32 AND L34
 L37 2051502 SEA FILE=HCAPLUS ABB=ON PLU=ON PHARMA?/SC,SX
 L38 1679 SEA FILE=HCAPLUS ABB=ON PLU=ON L37 AND L31
 L39 652504 SEA FILE=HCAPLUS ABB=ON PLU=ON PHARMACEU?/SC,SX
 L40 410 SEA FILE=HCAPLUS ABB=ON PLU=ON L39 AND L31
 L41 404 SEA FILE=HCAPLUS ABB=ON PLU=ON L39 AND L32
 L42 27 SEA FILE=HCAPLUS ABB=ON PLU=ON L35 AND L36 AND L38
 AND L40 AND L41
 L43 50 SEA FILE=HCAPLUS ABB=ON PLU=ON L42 OR L33

L45 93779 SEA FILE=HCAPLUS ABB=ON PLU=ON ESTROGEN?
L46 3741 SEA FILE=HCAPLUS ABB=ON PLU=ON L45 AND L31
L47 460 SEA FILE=HCAPLUS ABB=ON PLU=ON L15/THU
L48 12 SEA FILE=HCAPLUS ABB=ON PLU=ON L42 AND L47
L49 16 SEA FILE=HCAPLUS ABB=ON PLU=ON L46 AND L42
L50 17 SEA FILE=HCAPLUS ABB=ON PLU=ON L48 OR L49
L51 40 SEA FILE=HCAPLUS ABB=ON PLU=ON L50 OR L33
L54 10 SEA FILE=HCAPLUS ABB=ON PLU=ON L43 NOT L51
L55 5470 SEA FILE=HCAPLUS ABB=ON PLU=ON L31 AND 1840-1999/PY,P
RY
L56 9 SEA FILE=HCAPLUS ABB=ON PLU=ON L55 AND L54

=> d l56 1-9 ibib abs hitstr hitind

L56 ANSWER 1 OF 9 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1999:607548 HCAPLUS

DOCUMENT NUMBER: 131:337760

TITLE: Solubilization of hydrophobic compounds by
micellar solutions of hydrophobically modified
polyelectrolytes

AUTHOR(S): Bromberg, Lev; Temchenko, Marina

CORPORATE SOURCE: Department of Materials Science and
Engineering, Massachusetts Institute of
Technology, Cambridge, MA, 02139, USA

SOURCE: Langmuir (1999), 15(25), 8627-8632

CODEN: LANGD5; ISSN: 0743-7463

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Solubilization of pyrene and steroid hormones into aqueous solns. of
an associative polymer, poly(ethylene oxide)-b-poly(propylene
oxide)-b-(poly(ethylene oxide))-g-poly(acrylic acid)
(Pluronic-PAA), has been studied. A dramatic increase of
solubilization is observed upon formation of micelles above the critical
micellization temperature (cmt). The equilibrium partition coeffs. of the
probes between micelles and water (Km/w) above the cmt strongly
correlate with the probe's octanol/water partition coefficient (Ko/w).
The Km/w is increased with the ionization degree of the
poly(acrylic acid) (PAA) segments. Preferential solubilization of
the increasingly hydrophobic compds. into the Pluronic-PAA is
dominated by the entropic effect. Comparison of the fraction of
the probe located in the hydrophobic cores of the micellar
aggregates for pyrene and estradiol illustrates the degree of
chemical specificity of the Pluronic-PAA micellar aggregates, which
is due to the hydrophobicity of the probe.

IT 50-27-1, Estrinol

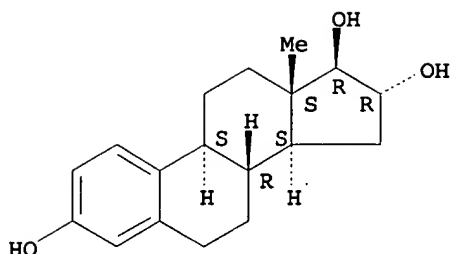
RL: PEP (Physical, engineering or chemical process); PRP
(Properties); PROC (Process)

(solubilization by micellar solns. of acrylic-grafted block
polyoxyalkylenes)

RN 50-27-1 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16,17-triol, (16 α ,17 β)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.



CC 37-5 (Plastics Manufacture and Processing)
 Section cross-reference(s): 32, 38, 62, 63

IT 50-27-1, Estriol 50-28-2, Estradiol, properties
 57-83-0, Progesterone, properties 58-22-0, Testosterone
 129-00-0, Pyrene, properties
 RL: PEP (Physical, engineering or chemical process); PRP
 (Properties); PROC (Process)
 (solubilization by micellar solns. of acrylic-grafted block
 polyoxyalkylenes)

REFERENCE COUNT: 56 THERE ARE 56 CITED REFERENCES AVAILABLE
 FOR THIS RECORD. ALL CITATIONS AVAILABLE
 IN THE RE FORMAT

L56 ANSWER 2 OF 9 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1997:289342 HCAPLUS
 DOCUMENT NUMBER: 127:900
 TITLE: Influence of the structure of steroid hormones
 on their association with cyclodextrins: a
 high-performance liquid chromatography study
 AUTHOR(S): Sadlej-Sosnowska, Nina
 CORPORATE SOURCE: Drug Institute, Warsaw, 00-725, Pol.
 SOURCE: Journal of Inclusion Phenomena and Molecular
 Recognition in Chemistry (1997),
 27(1), 31-40
 CODEN: JIMCEN; ISSN: 0923-0750

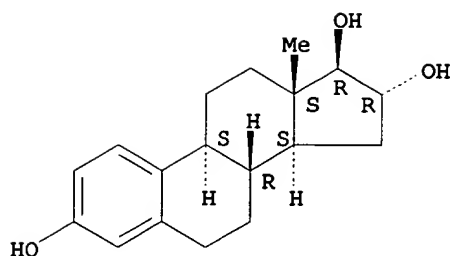
PUBLISHER: Kluwer
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB The association consts. of fourteen steroid hormones with β - and
 γ -cyclodextrin were measured in methanol-water (20:80
 volume/volume) at 35 °C using the chromatog. Hummel-Dreyer
 method. It was found that the greatest influence on the association
 consts. is the structural features of ring A of these compds. but
 the substituents of ring D also alter the complex stability to an
 appreciable degree. The measured association consts. were
 considerably greater than the corresponding values measured
 previously in the medium containing more methanol (45 instead of 20%).

IT 50-27-1, Estriol
 RL: PEP (Physical, engineering or chemical process); PROC
 (Process)
 (steroid hormone structure effect on association with cyclodextrins
 as detected by HPLC)

RN 50-27-1 HCAPLUS
 CN Estra-1,3,5(10)-triene-3,16,17-triol, (16 α ,17 β)- (9CI)
 (CA INDEX NAME)

Absolute stereochemistry.



CC 2-2 (Mammalian Hormones)

Section cross-reference(s): 32, 63

IT 50-02-2, Dexamethasone 50-24-8, Prednisolone 50-27-1,
 Estriol 50-28-2, Estradiol, processes 52-21-1, Prednisolone
 acetate 53-16-7, Estrone, processes 53-36-1,
 Methylprednisolone acetate 57-63-6, Ethinylestradiol 68-22-4,
 Norethisterone 83-43-2, Methylprednisolone 312-93-6,
 Dexamethasone phosphate 360-63-4, Betamethasone phosphate
 378-44-9, Betamethasone 434-22-0, Nandrolone 7585-39-9,
 β -Cyclodextrin 17465-86-0, γ -Cyclodextrin

RL: PEP (Physical, engineering or chemical process); PROC
 (Process)

(steroid hormone structure effect on association with cyclodextrins
 as detected by HPLC)

REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE
 FOR THIS RECORD. ALL CITATIONS AVAILABLE
 IN THE RE FORMAT

L56 ANSWER 3 OF 9 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1992:511878 HCAPLUS

DOCUMENT NUMBER: 117:111878

TITLE: NMR studies of estriol

AUTHOR(S): Ling, Yingzhi; Zhang, Zhiliang; Xu, Chunfang;
 Qiao, Liang

CORPORATE SOURCE: Dep. Pharm. Chem., Beijing Med. Univ.,
 Beijing, Peop. Rep. China

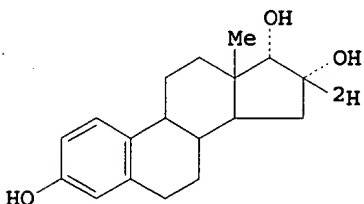
SOURCE: Beijing Yike Daxue Xuebao (1990),
 22(3), 213-4

CODEN: BYDXEV; ISSN: 1000-1530

DOCUMENT TYPE: Journal

LANGUAGE: Chinese

GI



I

AB The carbon-13 NMR spectrum of estriol was reported. Also reported
 were ATP (attached proton test) and HETCOR spectra of deuterated
 triol I.

IT 142886-39-3

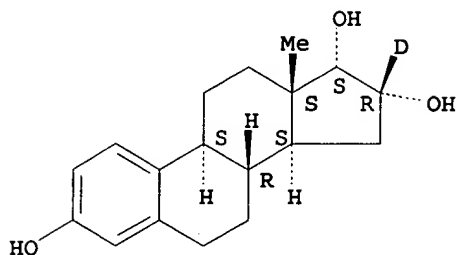
RL: PRP (Properties)
 (carbon-13 NMR spectra of)

RN 142886-39-3 HCAPLUS

CN Estra-1,3,5(10)-triene-16-d-3,16,17-triol, (16 α ,17 α)-

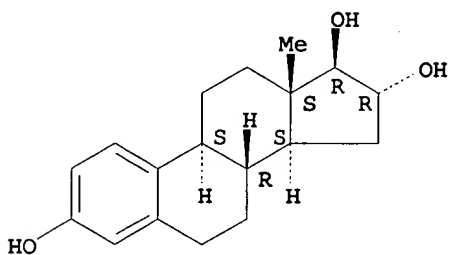
(9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 50-27-1, Estriol
 RL: PRP (Properties)
 (carbon-13 NMR spectrum of)
 RN 50-27-1 HCAPLUS
 CN Estra-1,3,5(10)-triene-3,16,17-triol, (16 α ,17 β)- (9CI)
 (CA INDEX NAME)

Absolute stereochemistry.



CC 32-3 (Steroids)
 Section cross-reference(s): 63, 77
 IT 142886-39-3
 RL: PRP (Properties)
 (carbon-13 NMR spectra of)
 IT 50-27-1, Estriol 7004-98-0
 RL: PRP (Properties)
 (carbon-13 NMR spectrum of)

L56 ANSWER 4 OF 9 HCAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 1992:476476 HCAPLUS
 DOCUMENT NUMBER: 117:76476
 TITLE: Crystallization method for steroids.
 INVENTOR(S): Lanquetin, Michel
 PATENT ASSIGNEE(S): Laboratoire Theramex S.A., Monaco
 SOURCE: PCT Int. Appl., 68 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: French
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9208730	A1	19920529	WO 1991-FR888	1991 1112

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W: BR, CA, FI, HU, JP, KR, SU, US
 RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LU, NL, SE
 FR 2668945 A1 19920515 FR 1990-13981

1990
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FR 2668945 B1 19930219
 CA 2073760 AA 19920513 CA 1991-2073760

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CA 2073760 C 20030923
 EP 510167 A1 19921028 EP 1992-900237

1991
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EP 510167 B1 19950823
 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE
 HU 61319 A2 19921228 HU 1992-2608

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 1112

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HU 212780 B 19961128
 BR 9106012 A 19930105 BR 1991-6012

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JP 05503305 T2 19930603 JP 1992-500415

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JP 3281954 B2 20020513
 ES 2079172 T3 19960101 ES 1992-900237

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RU 2126013 C1 19990210 RU 1991-5052919

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IL 101260 A1 19960119 IL 1992-101260

1992
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FI 9203188 A 19920710 FI 1992-3188

1992
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FI 111545 B1 20030815
 US 5266712 A 19931130 US 1992-910284

1992
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LV 11183 B 19961020 LV 1995-341

1995
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PRIORITY APPLN. INFO.: FR 1990-13981 A

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WO 1991-FR888 W

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 1112

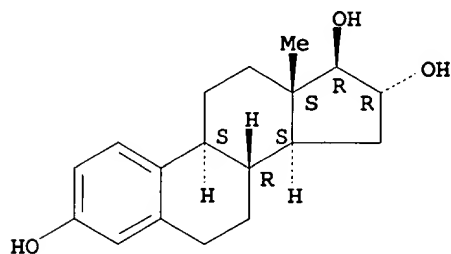
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AB A crystallization method is provided whereby a predetd. and homogeneous

particle size class can be obtained nonmech. A substance is dissolved in a ternary mixture consisting of a lipophilic solvent, a hydrophilic solvent and a surface-active agent at a temperature close to boiling. The mixture is allowed to cool to a temperature at which crystallization is initiated and the crystals formed are separated. Prednisone was refluxed in a mixture containing Me Et ketone 94.8, water 5.0, and Tween 20 0.2% until dissoln., then cooled at -10° to obtain microcrystals. A tablet contained above crystals 0.5, Avicel PH 102 50.00, Aerosil 1.70, Precirol ATO 5 2.00, and lactose to 130.00 mg.

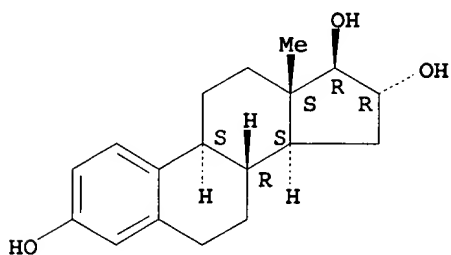
IT 50-27-1, Estriol 50-27-1D, Estriol, ethers and esters
 RL: PROC (Process)
 (crystallization of, for pharmaceutical formulations)
 RN 50-27-1 HCAPLUS
 CN Estra-1,3,5(10)-triene-3,16,17-triol, (16 α ,17 β)- (9CI)
 (CA INDEX NAME)

Absolute stereochemistry.



RN 50-27-1 HCAPLUS
 CN Estra-1,3,5(10)-triene-3,16,17-triol, (16 α ,17 β)- (9CI)
 (CA INDEX NAME)

Absolute stereochemistry.



IC ICM C07J001-00
 ICS A61K031-56; C07J005-00; C07J007-00; C07J011-00
 CC 63-5 (Pharmaceuticals)
 Section cross-reference(s): 32
 IT 50-02-2, Dexamethasone 50-02-2D, Dexamethasone, esters
 50-23-7, Hydrocortisone 50-27-1, Estriol
 50-27-1D, Estriol, ethers and esters 50-28-2, Estradiol,
 properties 50-28-2D, Estradiol, ethers and esters 53-03-2,
 Prednisone 53-06-5, Cortisone 53-06-5D, Cortisone, esters
 53-16-7, Estrone, properties 53-16-7D, Estrone, ethers and
 esters 14982-53-7D, Cholestane, derivs. 24749-37-9D, Estrane,
 derivs. 24887-75-0D, Androstane, derivs. 39219-28-8
 58652-20-3, Nomegestrol acetate 58691-88-6, Nomegestrol
 58691-88-6D, derivs. 58691-88-6D, Nomegestrol, esters
 102734-72-5D, 19-Nor-pregnane, derivs. 123505-24-8
 142715-46-6D, Pregn-4-en-21-ol, derivs. 142735-35-1

142761-13-5 142761-13-5D, ethers and esters
 RL: PROC (Process)
 (crystallization of, for pharmaceutical formulations)

L56 ANSWER 5 OF 9 HCAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 1992:449157 HCAPLUS
 DOCUMENT NUMBER: 117:49157
 TITLE: Preparation of brain-targeted
 acyloxymethylphosphonate prodrugs
 INVENTOR(S): Bodor, Nicholas S.
 PATENT ASSIGNEE(S): USA
 SOURCE: PCT Int. Appl., 179 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9200988	A1	19920123	WO 1991-US4824	1991 0712
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W: AT, AU, BB, BG, BR, CA, CH, CS, DE, DK, ES, FI, GB, HU, JP, KP, KR, LK, LU, MC, MG, MN, MW, NL, NO, PL, RO, SD, SE, SU				
RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FR, GA, GB, GN, GR, IT, LU, ML, MR, NL, SE, SN, TD, TG				
US 5177064	A	19930105	US 1990-553548	1990 0713
<--				
CA 2087194	AA	19920114	CA 1991-2087194	1991 0712
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AU 9183000	A1	19920204	AU 1991-83000	1991 0712
<--				
AU 649466	B2	19940526		
EP 539493	A1	19930505	EP 1991-913701	1991 0712
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EP 539493	B1	19970326		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE				
JP 05509313	T2	19931222	JP 1991-513064	1991 0712
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AT 150759	E	19970415	AT 1991-913701	1991 0712
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US 5413996	A	19950509	US 1992-962504	1992 1016
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US 5618803	A	19970408	US 1994-340896	1994 1115
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PRIORITY APPLN. INFO.:			US 1990-553548	A

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WO 1991-US4824

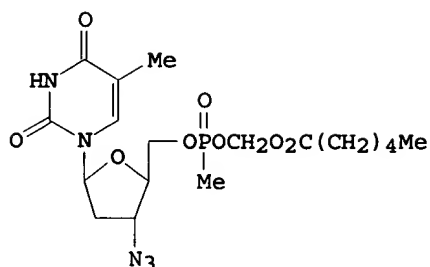
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US 1992-962504

A3

1992
1016

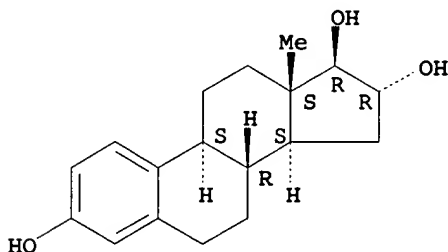
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OTHER SOURCE(S): MARPAT 117:49157
GI

II

- AB QP(O)(R1)OCHR2O2CR3 [Q = O-bonded drug moiety; R1 = alkyl, aryl, aralkyl; R2 = H, hetero)aryl, (cyclo)alkyl, heterocyclyl, aralkyl; R3 = alkyl, alkenyl, (alkyl)cycloalkyl(alkyl), aryloxyalkyl, pyridyl, (substituted) Ph, phenylalkyl], were prepared Thus, zidovudine was stirred with MeP(O)Cl2 and Na2CO3 in acetone for 17 h; H2O was added to give 31.3% zidovudine methylphosphonate (I), which was treated with iodomethyl hexanoate and CsF in DMF to give title compound II. Title compds. are rapidly hydrolyzed in vivo, and I was found in the brain after administration of II.
- IT 50-27-1DP, Estriol, acyloxymethylphosphonate derivative
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as brain-targeted prodrug)
- RN 50-27-1 HCAPLUS
- CN Estradiol, 1,3,5(10)-triene-3,16,17-triol, (16 α ,17 β)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.



- IC ICM C07H019-00
ICS C07J001-00; C07K001-00; A61K031-00; A61K033-00; A61K047-00
- CC 33-9 (Carbohydrates)
Section cross-reference(s): 1, 26, 32,
63
- IT 50-02-2DP, Dexamethasone, acyloxymethylphosphonate derivative
50-23-7DP, Hydrocortisone, acyloxymethylphosphonate derivative

50-24-8DP, Prednisolone, acyloxymethylphosphonate derivative
 50-27-1DP, Estriol, acyloxymethylphosphonate derivative
 50-28-2DP, Estradiol, acyloxymethylphosphonate derivative 50-50-ODP,
 Estradiol benzoate, acyloxymethylphosphonate derivative 50-89-5DP,
 Thymidine, acyloxymethylphosphonate derivative 50-91-9DP,
 acyloxymethylphosphonate derivative 52-76-6DP, Lynestrenol,
 acyloxymethylphosphonate derivative 53-03-2DP, Prednisone,
 acyloxymethylphosphonate derivative 53-06-5DP, Cortisone,
 acyloxymethylphosphonate derivative 53-16-7DP, Estrone,
 acyloxymethylphosphonate derivative 53-33-8DP, Paramethasone,
 acyloxymethylphosphonate derivative 53-34-9DP, Fluprednisolone,
 acyloxymethylphosphonate derivative 53-85-0DP,
 acyloxymethylphosphonate derivative 54-25-1DP, 6-Azaauridine,
 acyloxymethylphosphonate derivative 54-42-2DP, Idoxuridine,
 acyloxymethylphosphonate derivative 57-63-6DP, Ethinyl estradiol,
 acyloxymethylphosphonate derivative 58-18-4DP, Methyl testosterone,
 acyloxymethylphosphonate derivative 58-22-0DP, Testosterone,
 acyloxymethylphosphonate derivative 58-96-8DP, Uridine,
 acyloxymethylphosphonate derivative 61-32-5DP, Methicillin,
 silyloxymethylphosphonate derivative 61-33-6DP, Benzylpenicillin,
 silyloxymethylphosphonate derivative 61-72-3DP, Cloxacillin,
 silyloxymethylphosphonate derivative 66-79-5DP, Oxacillin,
 silyloxymethylphosphonate derivative 68-22-4DP, Norethindrone,
 acyloxymethylphosphonate derivative 70-00-8DP, Trifluridine,
 acyloxymethylphosphonate derivative 72-33-3DP, Mestranol,
 acyloxymethylphosphonate derivative 76-25-5DP, Triamcinolone
 acetone, acyloxymethylphosphonate derivative 79-64-1DP,
 Dimethisterone, acyloxymethylphosphonate derivative 83-43-2DP,
 Methyl prednisolone, acyloxymethylphosphonate derivative 87-08-1DP,
 Phenoxymethylpenicillin, silyloxymethylphosphonate derivative
 124-94-7DP, Triamcinolone, acyloxymethylphosphonate derivative
 127-31-1DP, Fludrocortisone, acyloxymethylphosphonate derivative
 147-52-4DP, Nafcillin, silyloxymethylphosphonate derivative
 147-94-4DP, Cytarabine, acyloxymethylphosphonate derivative
 152-43-2DP, Quinestrol, acyloxymethylphosphonate derivative
 152-58-9DP, Cortodoxone, acyloxymethylphosphonate derivative
 342-69-8DP, acyloxymethylphosphonate derivative 378-44-9DP,
 Betamethasone, acyloxymethylphosphonate derivative 432-60-0DP,
 Allylestrenol, acyloxymethylphosphonate derivative 434-03-7DP,
 Ethisterone, acyloxymethylphosphonate derivative 605-23-2DP, Ara-T,
 acyloxymethylphosphonate derivative 896-71-9DP, Tigestol,
 acyloxymethylphosphonate derivative 1035-77-4DP, Estradiol 3-methyl
 ether, acyloxymethylphosphonate derivative 1231-93-2DP, Ethynodiol,
 acyloxymethylphosphonate derivative 1247-42-3DP, Meprednisone,
 acyloxymethylphosphonate derivative 1476-82-0DP,
 acyloxymethylphosphonate derivative 1524-88-5DP, Flurandrenolide,
 acyloxymethylphosphonate derivative 2135-17-3DP, Flumethasone,
 acyloxymethylphosphonate derivative 3056-17-5DP,
 acyloxymethylphosphonate derivative 3083-77-0DP,
 acyloxymethylphosphonate derivative 3116-76-5DP, Dicloxacillin,
 silyloxymethylphosphonate derivative 3124-93-4DP, Ethynerone,
 acyloxymethylphosphonate derivative 3511-16-8DP, Hetacillin,
 silyloxymethylphosphonate derivative 3643-00-3DP, Oxogestone,
 acyloxymethylphosphonate derivative 4097-22-7DP,
 acyloxymethylphosphonate derivative 4697-36-3DP, Carbenicillin,
 silyloxymethylphosphonate derivative 5536-17-4DP, Vidarabine,
 acyloxymethylphosphonate derivative 6533-00-2DP, Norgestrel,
 acyloxymethylphosphonate derivative 6736-58-9DP, 3-Deazaadenosine,
 acyloxymethylphosphonate derivative 6795-60-4DP, Norvinisterone,
 acyloxymethylphosphonate derivative 7481-89-2DP, Dideoxycytidine,
 acyloxymethylphosphonate derivative 13563-60-5DP, Norgesterone,
 acyloxymethylphosphonate derivative 15176-29-1DP,
 acyloxymethylphosphonate derivative 16915-71-2DP, Cingestol,
 acyloxymethylphosphonate derivative 18417-89-5DP,
 acyloxymethylphosphonate derivative 23205-42-7DP, 3-Deazaauridine,
 acyloxymethylphosphonate derivative 25526-93-6DP,

acyloxymethylphosphonate derivative 26774-90-3DP, Epicillin,
 silyloxymethylphosphonate derivative 26787-78-ODP,
 silyloxymethylphosphonate derivative 30516-87-1DP, Zidovudine,
 acyloxymethylphosphonate derivative 31698-14-3DP, Cyclocytidine,
 acyloxymethylphosphonate derivative 34787-01-4DP, Ticarcillin,
 silyloxymethylphosphonate derivative 35943-35-2DP, Triciribine,
 acyloxymethylphosphonate derivative 36791-04-5DP, Ribavirin,
 acyloxymethylphosphonate derivative 41107-56-6DP,
 acyloxymethylphosphonate derivative 53910-25-1DP, Pentostatin,
 acyloxymethylphosphonate derivative 54262-83-8DP,
 acyloxymethylphosphonate derivative 56039-11-3DP, 3-Deazaguanosine,
 acyloxymethylphosphonate derivative 58316-88-4DP,
 3-Deazaaristeromycin, acyloxymethylphosphonate derivative
 59277-89-3DP, Acyclovir, acyloxymethylphosphonate derivative
 60084-10-8DP, Tiazofurin, acyloxymethylphosphonate derivative
 69123-90-6DP, FIAC, acyloxymethylphosphonate derivative
 69123-98-4DP, FIAU, acyloxymethylphosphonate derivative
 69256-17-3DP, acyloxymethylphosphonate derivative 69304-47-8DP,
 BVDU, acyloxymethylphosphonate derivative 69655-05-6DP,
 Dideoxyinosine, acyloxymethylphosphonate derivative 69979-46-ODP,
 Cyclaradine, acyloxymethylphosphonate derivative 72877-50-ODP,
 acyloxymethylphosphonate derivative 82410-32-ODP, Ganciclovir,
 acyloxymethylphosphonate derivative 83546-42-3DP,
 acyloxymethylphosphonate derivative 83705-13-9DP, Selenazofurin,
 acyloxymethylphosphonate derivative 84408-37-7DP, 6-Deoxyacyclovir,
 acyloxymethylphosphonate derivative 85236-92-6DP,
 acyloxymethylphosphonate derivative 86304-28-1DP, Buciclovir,
 acyloxymethylphosphonate derivative 90301-59-ODP,
 acyloxymethylphosphonate derivative 105784-82-5DP,
 acyloxymethylphosphonate derivative 114522-22-4DP,
 acyloxymethylphosphonate derivative 119644-22-3DP,
 acyloxymethylphosphonate derivative 119770-71-7DP,
 acyloxymethylphosphonate derivative 119770-72-8DP,
 acyloxymethylphosphonate derivative 142118-61-4P 142118-62-5P
 142118-63-6P 142118-64-7P 142118-65-8DP,
 acyloxymethylphosphonate derivative 142186-29-6DP,
 acyloxymethylphosphonate derivative 142186-30-9DP,
 acyloxymethylphosphonate derivative
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of, as brain-targeted prodrug)

L56 ANSWER 6 OF 9 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1990:446267 HCAPLUS
 DOCUMENT NUMBER: 113:46267
 TITLE: Pharmaceutical formulations for parenteral use
 containing cyclodextrins and dihydropyridine
 redox systems
 INVENTOR(S): Bodor, Nicholas S.
 PATENT ASSIGNEE(S): University of Florida, USA
 SOURCE: Eur. Pat. Appl., 125 pp.
 CODEN: EPXXDW
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 2
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 335545	A2	19891004	EP 1989-302719	1989 0320
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EP 335545	A3	19900926		
EP 335545	B1	19930609		
EP 335545	B2	19980923		

R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE
 US 4983586 A 19910108 US 1988-174945

1988
 0329

EP 327766 A2 19890816 EP 1988-312016

1988
 1219

EP 327766 A3 19900926

EP 327766 B1 19980408

R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE

AT 90200 E 19930615 AT 1989-302719

1989
 0320

AU 8931762 A1 19890727 AU 1989-31762

1989
 0328

AU 618995 B2 19920116

CA 1336498 A1 19950801 CA 1989-594911

1989
 0328

JP 02009825 A2 19900112 JP 1989-77938

1989
 0329

JP 2643426 B2 19970820

ZA 8902315 A 19901228 ZA 1989-2315

1989
 0329

US 5017566 A 19910521 US 1989-431222

1989
 1103

US 5024998 A 19910618 US 1989-448655

1989
 1211

PRIORITY APPLN. INFO.:

US 1988-174945

A

1988
 0329

EP 1988-312016

A

1988
 1219

US 1987-139755

A2

1987
 1230

CA 1988-585791

A

1988
 1213

IE 1988-3717

A

1988
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IE 1989-810

A

1989
 0314

EP 1989-302719 A
1989
0320

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US 1989-431222 A2
1989
1103

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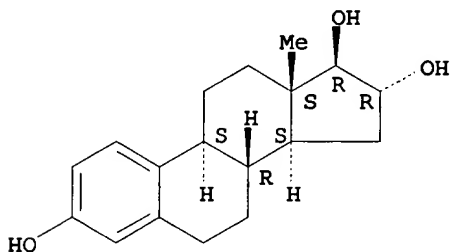
AB Aqueous parenteral solns. of drugs which are insol. or only sparingly soluble and/or which are unstable in water, are combined with a cyclodextrin derivative to provide a means for alleviating problems associated with drug precipitation at the injection site and/or in the lungs or other organs following parenteral administration. Another approach is use of the dihydropyridine-pyridinium redox delivery system. A large number of examples are given for synthesis of dihydropyridine and pyridinium derivs. of drugs. Data are also presented showing drug solubilization by cyclodextrin derivs.

IT 50-27-1, Estriol
RL: PRP (Properties)
(parenteral delivery systems containing cyclodextrins or pyridine redox systems of)

RN 50-27-1 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16,17-triol, (16 α ,17 β)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.



IC ICM A61K009-08

ICS A61K047-00

CC 63-5 (Pharmaceuticals)

Section cross-reference(s): 1, 27, 28, 32, 33

IT 50-02-2, Dexamethasone 50-06-6, Phenobarbital, biological studies 50-23-7, Hydrocortisone 50-24-8 50-27-1, Estriol 50-28-2, 17 β -Estradiol, biological studies 50-44-2, Mercaptopurine 50-47-5, Desipramine 50-50-0, Estradiol benzoate 51-21-8, 5-Fluorouracil 51-61-6, Dopamine, biological studies 51-98-9 52-01-7, Spironolactone 53-16-7, Estrone, biological studies 53-86-1, Indomethacin 54-31-9, Furosemide 55-63-0, Nitroglycerin 56-12-2, GABA, biological studies 57-41-0, Phenytoin 57-63-6 57-83-0, Progesterone, biological studies 58-00-4, Apomorphine 58-18-4, 17-Methyltestosterone 58-22-0, Testosterone 58-25-3, Chlordiazepoxide 59-05-2, Methotrexate 59-66-5, Acetazolamide 59-92-7, L-DOPA, biological studies 60-18-4, Tyrosine, biological studies 61-32-5, Methicillin 61-33-6, Benzylpenicillin, biological studies 61-54-1, Tryptamine 61-72-3, Cloxacillin 66-76-2, Dicumarol 66-79-5, Oxacillin 67-52-7D, Barbituric acid, derivs. 68-22-4 68-23-5, Norethynodrel 68-26-8, Retinol 69-53-4, Ampicillin 70-00-8, Trifluorothymidine 71-58-9, Medroxyprogesterone acetate 71-63-6, Digitoxin 72-33-3, Mestranol 76-73-3, Secobarbital 76-74-4 77-36-1, Chlorthalidone 99-66-1, Valproic acid 116-31-4, Retinal 127-47-9, Vitamin A acetate 137-58-6, Lidocaine 148-82-3, Melphalan 154-93-8, Car mustine

305-03-3, Chlorambucil 434-03-7 439-14-5, Diazepam 512-64-1,
 Echinomycin 523-87-5, Dimenhydrinate 604-75-1, Oxazepam
 645-05-6, Hexamethylmelamine 745-65-3, Alprostadil 846-49-1,
 Lorazepam 968-81-0, Acetohexamide 1406-16-2, Vitamin D
 1406-18-4, Vitamin E 2365-30-2 2898-12-6, Medazepam
 3116-76-5, Dicloxacillin 5104-49-4, Flurbiprofen 6533-00-2,
 Norgestrel 8064-90-2, Co-trimoxazole 12001-79-5, Vitamin K
 12794-10-4D, Benzodiazepine, derivs. 13010-47-4, Lomustine
 13182-89-3, Metronidazole benzoate 13909-02-9, PCNU
 13909-09-6, Semustine 15676-16-1, Sulpiride 20830-75-5,
 Digoxin 22204-53-1, Naproxen 22916-47-8 23930-19-0,
 Alfaxalone 29767-20-2, Teniposide 30516-87-1 31430-15-6,
 Flubendazole 33125-97-2, Etomidate 33419-42-0, Etoposide
 35121-78-9, Prostacyclin 36322-90-4, Piroxicam 41451-75-6,
 Bruceantin 51264-14-3, Amsacrine 52468-60-7, Flunarizine
 57998-68-2, Diaziquone 59277-89-3, Acyclovir 61422-45-5,
 Carmofur 65277-42-1, Ketoconazole 65886-71-7, Fazarabine
 69112-98-7 77327-05-0, Didemnin B 84625-61-6 84697-22-3
 127950-65-6

RL: PRP (Properties)

(parenteral delivery systems containing cyclodextrins or pyridine
 redox systems of)

L56 ANSWER 7 OF 9 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1987:464732 HCAPLUS

DOCUMENT NUMBER: 107:64732

TITLE: Thermoanalytical study of some steroids. I.
 Estradiol monovalerate and estriol

AUTHOR(S): De Maury, G.; Masse, J.

CORPORATE SOURCE: Lab. Chim. Gen. Miner., Fac. Pharm.,
 Montpellier, 34060, Fr.

SOURCE: Journal of Thermal Analysis (1986),
 31(6), 1263-77

CODEN: JTSEA9; ISSN: 0368-4466

DOCUMENT TYPE: Journal

LANGUAGE: French

AB A thermoanal. study of estradiol monovalerate (I) and estriol (II)
 showed the thermal stability, the decomposition kinetics, and the
 temps. and intervals of fusion. The degree of purity was calculated
 only for I: 99.72 mol %. The fusion enthalpy (29.45 kJ mol⁻¹) and
 entropy for I were evaluated by DSC. It was also possible to
 detect the polymorphism and the pseudopolymorphism of I and II
 after recrystn. from several solvents.

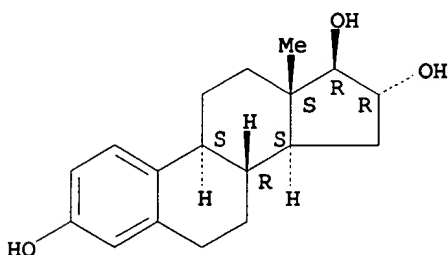
IT 50-27-1, Estriol

RL: PROC (Process)
 (thermal anal. of)

RN 50-27-1 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16,17-triol, (16 α ,17 β)- (9CI)
 (CA INDEX NAME)

Absolute stereochemistry.



CC 63-5 (Pharmaceuticals)

Section cross-reference(s): 22, 32

IT 50-27-1, Estriol 27811-56-9, Estradiol monovalerate
 RL: PROC (Process)
 (thermal anal. of)

L56 ANSWER 8 OF 9 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1985:46183 HCAPLUS

DOCUMENT NUMBER: 102:46183

TITLE: Diethylsilyl ether and diethylsiliconide derivatives in gas chromatography/mass spectrometry of hydroxylated steroids

AUTHOR(S): Miyazaki, Hiroshi; Ishibashi, Masataka; Itoh, Masahiro; Yamashita, Kouwa

CORPORATE SOURCE: Res. Lab., Nippon Kayaku Co., Tokyo, 115, Japan

SOURCE: Biomedical Mass Spectrometry (1984), 11(8), 377-82

CODEN: BMSYAL; ISSN: 0306-042X

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The gas chromatog. and mass spectrometric properties of the diethylsilyl (DEHS) or diethylsiliconide (DES)-DEHS ether derivs. of 20 hydroxysteroids of various types have been studied using N,O-bis(diethylsilyl)trifluoroacetamide as a new silylating agent. The mass spectra of the DES-DEHS ether derivs. were characterized by their marked simplicity and by mol. ions of high abundance, whereas the mass fragmentation patterns of the DEHS ether derivs. without formation of the DES group in the mol. were similar to those of the corresponding dimethylethylsilyl (DMES) ether derivs. The appearance of the mol. ion may be very useful for estimating the mol. weight of hydroxysteroids of which other silyl ether derivs. yield mol. ions of insufficient abundance to characterize them. In particular, the DES-DEHS ether derivative of 5 β -pregnane-3 α ,17 α ,20 α -triol gave the mol. ion at m/z 506 as a principal ion in the electron-impact ionization mode. The methylene unit values of the DEHS ether derivs. of hydroxysteroids without formation of DES groups were slightly larger than those of the corresponding DMES ether derivs. A $\Delta[U_m]$ s value was presented for estimation of the number of siliconide moieties in the DES-DEHS ether derivs.

IT 50-27-1D, diethylsilyl ethers and diethylsiliconide derivs. 547-81-9D, diethylsilyl ethers and diethylsiliconide derivs. 1228-72-4D, diethylsilyl ethers and diethylsiliconide derivs. 15183-37-6D, diethylsilyl ethers and diethylsiliconide derivs.

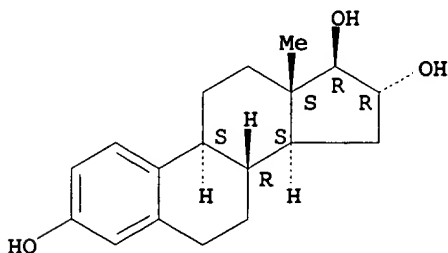
RL: PRP (Properties)

(gas chromatog.-mass spectrum of)

RN 50-27-1 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16,17-triol, (16 α ,17 β)- (9CI)
 (CA INDEX NAME)

Absolute stereochemistry.

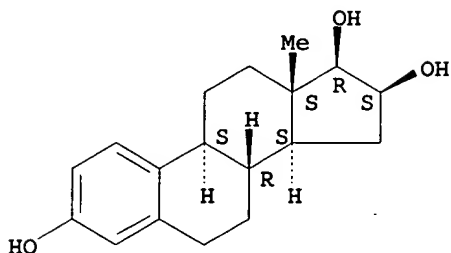


RN 547-81-9 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16,17-triol, (16 β ,17 β)- (9CI)

(CA INDEX NAME)

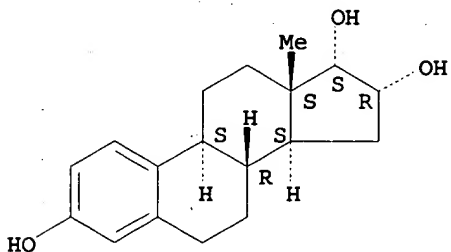
Absolute stereochemistry.



RN 1228-72-4 HCAPLUS

CN. Estra-1,3,5(10)-triene-3,16,17-triol, (16 α ,17 α)- (9CI)
(CA INDEX NAME)

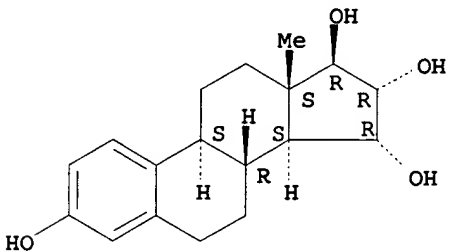
Absolute stereochemistry.



RN 15183-37-6 HCAPLUS

CN. Estra-1,3,5(10)-triene-3,15,16,17-tetrol,
(15 α ,16 α ,17 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



CC 32-5 (Steroids)

Section cross-reference(s): 64

IT 50-27-1D, diethylsilyl ethers and diethylsiliconide

derivs. 50-28-2D, diethylsilyl ethers and diethylsiliconide

derivs. 53-16-7D, diethylsilyl ethers and diethylsiliconide

derivs. 53-43-0D, diethylsilyl ethers and diethylsiliconide

derivs. 58-22-0D, diethylsilyl ethers and diethylsiliconide

derivs. 80-89-7D, diethylsilyl ethers and diethylsiliconide

derivs. 80-92-2D, diethylsilyl ethers and diethylsiliconide

derivs. 80-97-7D, diethylsilyl ethers and diethylsiliconide

derivs. 481-30-1D, diethylsilyl ethers and diethylsiliconide

derivs. 516-53-0D, diethylsilyl ethers and diethylsiliconide

derivs. 516-95-0D, diethylsilyl ethers and diethylsiliconide

derivs. 520-86-5D, diethylsilyl ethers and diethylsiliconide

derivs. 547-81-9D, diethylsilyl ethers and diethylsiliconide derivs. 566-58-5D, diethylsilyl ethers and diethylsiliconide derivs. 570-50-3D, diethylsilyl ethers and diethylsiliconide derivs. 1098-45-9D, diethylsilyl ethers and diethylsiliconide derivs. 1228-72-4D, diethylsilyl ethers and diethylsiliconide derivs. 1851-23-6D, diethylsilyl ethers and diethylsiliconide derivs. 1852-53-5D, diethylsilyl ethers and diethylsiliconide derivs. 15183-37-6D, diethylsilyl ethers and diethylsiliconide derivs.
 RL: PRP (Properties)
 (gas chromatog.-mass spectrum of)

L56 ANSWER 9 OF 9 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1972:49943 HCAPLUS
 DOCUMENT NUMBER: 76:49943
 TITLE: Inducing ovulation with compositions comprising 13-alkyl-16 α -hydroxy-3,17-dioxygenated-gona-1,3,5(10)-trienes
 INVENTOR(S): Edgren, Richard A.
 PATENT ASSIGNEE(S): American Home Products Corp.
 SOURCE: U.S., 5 pp.
 CODEN: USXXAM
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

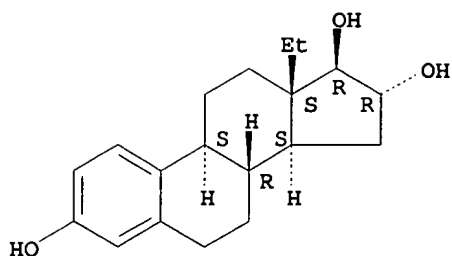
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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US 3622670	A	19711123	US 1969-852447	1969 0822

PRIORITY APPLN. INFO.: <--
 US 1969-852447 A 1969
 0822

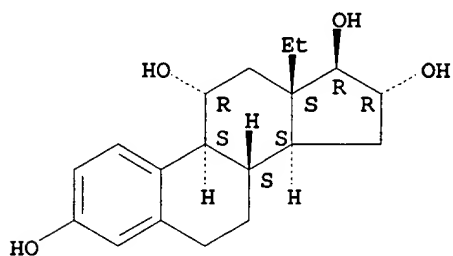
GI For diagram(s), see printed CA Issue.
 AB 13-Ethylgona-1,3,5(10)-triene-3,16 α ,17 β -triol (I) and a carrier were used to induce ovulation in warm-blooded anovulatory vertebrates after administration. I was prepared by LiAlH₄ reduction of 3,17-diacetoxy-16 α ,17 α -epoxy-1,3,5(10)-triene (II) followed by treatment with EtOAc and 2N HCl. In an example, tablets were prepared from I 5, CM-cellulose 15, lactose 25, redried corn starch 25, Mg stearate 4 mg, and sufficient Ca silicate to give 200 mg of tablet.
 IT 19882-03-2 36292-12-3 36292-13-4
 RL: BIOL (Biological study)
 (for ovulation induction)
 RN 19882-03-2 HCAPLUS
 CN Gona-1,3,5(10)-triene-3,16,17-triol, 13-ethyl-, (16 α ,17 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



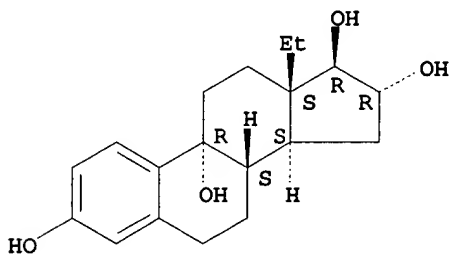
RN 36292-12-3 HCAPLUS
 CN Gona-1,3,5(10)-triene-3,11,16,17-tetrol, 13-ethyl-,
 (11 α ,16 α ,17 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 36292-13-4 HCAPLUS
 CN Gona-1,3,5(10)-triene-3,9,16,17-tetrol, 13-ethyl-,
 (16 α ,17 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IC A61K
 INCL 424238000
 CC 63 (Pharmaceuticals)
 Section cross-reference(s): 32
 IT 1474-53-9 18318-03-1 18318-06-4 18318-07-5
 19882-03-2 36292-12-3 36292-13-4
 RL: BIOL (Biological study)
 (for ovulation induction)

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